The General Setting for Shape Deformation Analysis and LDDMM

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A Brief Summary of LDDMM

Purpose of LDDMM: Compare two "shapes" q_0 and q_1 in $\mathbb{R}^d$ in a way that takes into account their **geometric properties** (smoothness, self-intersection...). The initial shape q_0 is the **template**, q_1 is the **target**.

Examples of shapes:

- Landmarks: $q = (x_1, \dots x_n)$, $x_i \in \mathbb{R}^d$
- Parametrized embedded curves, surfaces and submanifolds: $q \in \mathrm{Emb}^k(M, \mathbb{R}^d)$
- Unparametrized embedded curves, surfaces and submanifolds: $q \in \mathrm{Emb}^k(M, \mathbb{R}^d)/\mathcal{D}^k(M)$ **(Bauer, Bruveris, Michor)**

A Brief Summary of LDDMM

Method: Let $(V, \langle \cdot, \cdot \rangle)$ be a Hilbert space of vector fields with continuous inclusion in $\mathcal{C}^1_0(\mathbb{R}^d, \mathbb{R}^d)$. A time-dependent vector field $v \in L^2(0,1; V)$ admits a unique flow $\varphi(\cdot)$ such that

$$\partial_t \varphi(t,x) = v(t, \varphi(t,x)), \quad t \in [0,1],\ x \in \mathbb{R}^d,$$

which acts on the template q_0 (composition on the left), deforming it into

$$q(t) = \varphi(t) \cdot q_0,$$

yielding the infinitesimal action

$$\dot{q}(t) = v(t) \cdot q(t).$$

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Then, minimize

$$J(v) = \frac{1}{2}\int_0^1 \|v(t)\|_V^2 dt + g(q(1)).$$

with g data attachment that gets smaller the closer $q(1)$ gets to q_1, and

$$q(0) = q_0, \quad \dot{q}(t) = v(t) \cdot q(t).$$

We have examples of shapes and shape spaces, but no general definition. What if we want to track a vector field along the shape (muscle fibers)? Or shapes with parts of different dimensions?

Key remark: we only need an action of $\mathcal{D}(\mathbb{R}^d)$ (that satisfies certain properties) to apply the LDDMM method.

Plan

1. The Group Structure of Diffeomorphisms
2. Shape Spaces

Plan

1 The Group Structure of Diffeomorphisms

2 Shape Spaces

Diffeomorphisms of Sobolev regularity

Fix $s > d/2 + 1$ integer. Then **(Bruveris, Vialard)**

$$\mathcal{D}^s(\mathbb{R}^d) = \left(\mathrm{Id}_{\mathbb{R}^d} + H^s(\mathbb{R}^d, \mathbb{R}^d)\right) \cap \mathcal{D}(\mathbb{R}^d)$$

is a Hilbert manifold (open subset of an affine Hilbert space) and a topological group for $(\varphi, \psi) \mapsto \varphi \circ \psi$.

Right composition: $R_\psi : \varphi \mapsto \varphi \circ \psi$ is of class $\mathcal{C}^\infty$
$\Rightarrow$ for $v \in H^s(\mathbb{R}^d, \mathbb{R}^d)$, right-invariant "vector field" **on** $\mathcal{D}^s(\mathbb{R}^d)$
$\mathbf{v}(\varphi) = dR_\varphi(v) = v \circ \varphi$.

Left composition: $(\varphi, \psi) \mapsto \varphi \circ \psi$ (resp. $(v, \varphi) \mapsto v \circ \varphi$) is of class $\mathcal{C}^k$ when restricted to $\mathcal{D}^{s+k}(\mathbb{R}^d) \times \mathcal{D}^s(\mathbb{R}^d)$ (resp. $H^{s+k}(\mathbb{R}^d, \mathbb{R}^d) \times \mathcal{D}^s(\mathbb{R}^d)$).

Control Space For LDDMM

Towards LDDMM: Fix $(V, \langle \cdot, \cdot \rangle)$ Hilbert space of vector fields with continuous inclusion in $H^s(\mathbb{R}^d, \mathbb{R}^d)$.

Now $v \in L^2(0, 1; V)$ gives rise to a unique flow, a curve $\varphi(\cdot) \in H^1(0, 1; \mathcal{D}^s(\mathbb{R}^d))$ by solving the **control system**

$$\varphi(0) = \mathrm{Id}_{\mathbb{R}^d}, \quad \dot{\varphi}(t) = v(t) \circ \varphi(t), \quad t \in [0, 1].$$

This flow has energy $E(\varphi) = E(v) = \frac{1}{2} \int_0^1 \|v(t)\|^2 dt$.

Distance

$\Longrightarrow$ We can define the length, then the distance d_V between two diffeomorphisms induced by this V. This is a **Sub-Riemannian structure** on $\mathcal{D}^s(\mathbb{R}^d)$.

Proposition 1 (Trouvé)

The metric space $(\mathcal{D}^s(\mathbb{R}^d), d_V)$ is complete. Moreover, if $d(\varphi, \psi) < +\infty$, they can be connected by a geodesic.

Geodesics

Question: what are the geodesics (i.e., minimizers of energy with fixed endpoints): Optimal Control.

Problem: no Pontryagin Maximum Principle (PMP) in infinite dimensions: no (workable) necessary condition! However, we still have sufficient conditions.

Hamiltonian

- Let $K_V : V^* \to V$ be the Riesz operator. Any

$$P \in H^s(\mathbb{R}^d, \mathbb{R}^d)^* = H^{-s}(\mathbb{R}^d, \mathbb{R}^d)$$

  also belongs to V^*: $K_V P \in V$.

- K_V is given by convolution with a kernel $K : \mathbb{R}^d \times \mathbb{R}^d \to M_d(\mathbb{R})$:

$$K_V P(x) = \int_{\mathbb{R}^d} K(x, y)P(y)dy.$$

- **Hamiltonian:** $dR_\varphi^* P$ given by $(dR_\varphi^* P|v) = (P|v \circ \varphi)$. The Hamiltonian of the system is

$$H(\varphi, P) = \frac{1}{2}\|K_V dR_\varphi^* P\|^2 = \frac{1}{2}\iint_{\mathbb{R}^d \times \mathbb{R}^d} P(x) \cdot K(\varphi(x), \varphi(y))P(y)dydx.$$

Theorem 1

Assume V has continuous inclusion in $H^{s+2}(\mathbb{R}^d,\mathbb{R}^d)$. Then the **Hamiltonian geodesic flow**

$$\begin{cases} \partial_t\varphi(t,x) = \partial_P H(\varphi(t),P(t))(x) & = v(t,\varphi(t,x)), \\ \partial_t P(t,x) = -\partial_\varphi H(\varphi(t),P(t))(x) & = -dv(t,\varphi(t,x))^T P(t,x), \end{cases}$$

where

$$v(t,x) = \int_{\mathbb{R}^d} K(x,\varphi(t,y))P(t,y)dy = K_V dR^*_{\varphi(t)}P(t),$$

is complete, and the corresponding curves $t\mapsto\varphi(t)$ are geodesics on small enough intervals.

Important remark: some geodesics may not appear in the Hamiltonian flow, so this is a sufficient condition, not a necessary condition.

Momentum Viewpoint

Define the **momentum map** $\mu(\varphi, P) = dR_\varphi^* P \in H^{-s}(\mathbb{R}^d, \mathbb{R}^d)$.

Proposition 2 (Euler-Poincarré)

A curve $t \mapsto (\varphi(t), P(t))$ follows the Hamiltonian flow if and only if its momentum $\mu(t) = \mu(\varphi(t), P(t))$ satisfies

$$\dot{\mu}(t) = -ad^*_{K_V \mu(t)} \mu(t),$$

where $ad_v w = -[v, w]$, which integrates into

$$\mu(t) = \varphi_* \mu(0).$$

In particular, the regularity of μ is preserved along the trajectory and $\operatorname{supp} \mu(t) = \varphi(t)(\operatorname{supp} \mu(0))$.

For example, if $\mu(0)$ is a sum of n vector-valued Dirac masses, so is $\mu(t)$ for every time t.

Remark: In general, the equation **cannot** be converted into the Arnol'd equation

$$\dot{v}(t) = -ad_{v(t)}^T v(t)$$

through $v(t) = K_V \mu(t)$. For example, different $\mu(0)$ can yield the same $v(0)$ but not the same $v(t)$.

Plan

1 The Group Structure of Diffeomorphisms

2 Shape Spaces

Definition

Let $\mathcal{S}$ be a Banach manifold, fix $\ell \in \mathbb{N}$, and s_0 the smallest integer such that $s_0 > d/2$. Let $s = s_0 + \ell$. A continuous action $(\varphi, q) \mapsto \varphi \cdot q$ of $\mathcal{D}^s(M)$ on $\mathcal{S}$ makes it into a **shape space of order** ℓ if:

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- For any $q \in \mathcal{S}$ fixed, $R_q : \varphi \mapsto \varphi \cdot q$ is of class $\mathcal{C}^\infty$. We then define the **infinitesimal action** ξ of $v \in H^s(\mathbb{R}^d, \mathbb{R}^d)$ by $\xi_q v := dR_q(\mathrm{Id}_{\mathbb{R}^d})v$.

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- For every $k \geq 1$, the following mappings are $\mathcal{C}^k$:

$$\begin{aligned} \mathcal{D}^{s+k}(\mathbb{R}^d) \times \mathcal{S} &\to \mathcal{S} \\ (\varphi, q) &\mapsto \varphi \cdot q \end{aligned} \qquad \begin{aligned} H^{s+k}(\mathbb{R}^d, \mathbb{R}^d) \times \mathcal{S} &\to T\mathcal{S} \\ (v, q) &\mapsto \xi_q v \end{aligned}$$

Examples

- All classical examples (landmark spaces, embedding spaces, spaces of submanifolds) are shape spaces of varying order (0 for landmarks, ℓ for $\mathcal{C}^\ell$-embeddings,...).
- $\mathcal{D}^{s_0+\ell}(\mathbb{R}^d)$ is itself a shape space of order ℓ (in a way, it's the biggest).
- So is the product of any two shape spaces (which yields unions of shapes with different dimensions).
- If $\mathcal{S}$ is a shape space of order ℓ, $T\mathcal{S}$ is a shape space of order $\ell+1$ (application: shapes with fibers).

The space of images $L^2(\mathbb{R}^d)$ with action $\varphi \cdot I = I \circ \varphi^{-1}$ is **not** a shape space. However, this case can still be treated with our method.

The general LDDMM problem

- Fix a Hilbert space of vector fields V with continuous inclusion in $H^s(\mathbb{R}^d, \mathbb{R}^d)$. Fix a template q_0 and let $g : \mathcal{S} \to \mathbb{R}$ be a data attachment term of class $\mathcal{C}^1$.

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- Fix a Hilbert space of vector fields V with continuous inclusion in $H^s(\mathbb{R}^d, \mathbb{R}^d)$. Fix a template q_0 and let $g : \mathcal{S} \to \mathbb{R}$ be a data attachment term of class $\mathcal{C}^1$.
- We wish to minimize

$$J(v) = \frac{1}{2}\int_0^1 \|v(t)\|^2 dt + g(q(1))$$

over $v \in L^2(0,1;V)$, where $q(\cdot)$ is the trajectory of the sub-Riemannian control system

$$q(0) = q_0, \quad \dot{q}(t) = \xi_{q(t)} v(t) \quad (\Leftrightarrow q(t) = \varphi(t) \cdot q_0).$$

Push-forward of the Hamiltonian flow

Theorem 2

Assume that V has continuous inclusion in $H^{s+1}(\mathbb{R}^d, \mathbb{R}^d)$.

Then a control v is a critical point of J if and only if the flow of v is the projection of a Hamiltonian geodesic on $\mathcal{D}^s(\mathbb{R}^d)$ with final momentum $\mu(1) = \xi^*_{q(1)} dg(q(1))$.

Moreover, $\mu(t) = \xi^*_{q(t)} p(t)$ for some $p(t) \in T^*_{q(t)}\mathcal{S}$.

We get $v(t) = K_V \xi^*_{q(t)} p(t)$ and

$$\dot{q}(t) = \xi_{q(t)} K_V \xi^*_{q(t)} p(t) =: K_{q(t)} p(t).$$

Hamiltonian flow on $\mathcal{S}$

Letting

$$H^{\mathcal{S}}(q,p) = \frac{1}{2}(p|K_q p),$$

we just get $p(1) + dg(q(1)) = 0$, and

$$\dot{q}(t) = \partial_p H^{\mathcal{S}}(q(t), p(t)), \quad \dot{p}(t) = -\partial_p H^{\mathcal{S}}(q(t), p(t)).$$

Reduction

Important Application: we can simply minimize

$$\frac{1}{2}\int_0^1 (p(t)|K_{q(t)}p(t))dt + g(q(1)), \quad \dot{q}(t) = K_{q(t)}p(t),$$

finite dimensional optimal control problem in numerical applications.

Further reductions possible, for example if g and ξ are invariant under the action of some other group G (reparametrizetion of an embedded manifold for example).

Images

When matching a smooth template image I_0 onto a target I_1, we can simply consider the entire $\mathcal{D}^s(\mathbb{R}^d)$ as a shape space, with data attachment $g(\varphi) = \|I_0 \circ \varphi^{-1} - I_1\|_{L^2}^2$. A change of variable easily shows that g is of class $\mathcal{C}^1$, and we can apply our method.

This will reprove the well-known fact that, for LDDMM image matching, the momentum $\mu(t)$ at time t is pointwise colinear with the gradient in space of $I(t) = I_0 \circ \varphi(t)^{-1}$:

$$\mu(t) = (I(t) - I_1 \circ \varphi(1-t))\partial_x I(t).$$

Thank you for your attention!