The Abstract Setting for Shape Deformation Analysis and LDDMM Methods

Sylvain Arguillère(✉)

Johns Hopkins University, Baltimore, MD, USA
sarguil1@johnshopkins.edu

Abstract. This paper aims to define a unified setting for shape registration and LDDMM methods for shape analysis. This setting turns out to be sub-Riemannian, and not Riemannian. An abstract definition of a space of shapes in $\mathbb{R}^d$ is given, and the geodesic flow associated to any reproducing kernel Hilbert space of sufficiently regular vector fields is showed to exist for all time.

1 Introduction

The purpose of this paper is to define and study abstract shape spaces in $\mathbb{R}^d$ in order to unify and generalize the LDDMM algorithms that have been developed in the past few years. They consist in fixing a Hilbert space V of smooth vector fields in $\mathbb{R}^d$ with reproducing kernel K, and studying the deformations of an initial shape (a *template*) induced by flows of elements of V [8,10,17–21]. This allows to measure the "energy" of this flow by integrating the squared norm of the vector field. One then tries to get as close as possible to a target shape while keeping the energy small. This induces a length structure on the shape space and the problem can be reformulated as a geodesic search for this structure.

However, these methods have some flaws from a theoretical point of view. First of all, the notion of "shape space" has always been ambiguous. While it usually refers to a space of embeddings of a compact surface in $\mathbb{R}^3$ (or, in numerical simulations, to spaces of landmarks), more general spaces are sometimes needed and therefore require a case by case analysis. For example, when studying the movement of a muscle, one needs to take into account the direction of that muscle's fibers, which are not part of the embedding itself.

The second problem only appears for a shape space $\mathcal{S}$ of infinite dimension. Contrarily to what is described in most papers, the length structure induced by the flow of vector fields in V yields a *sub-Riemannian structure* on $\mathcal{S}$, not a Riemannian one. While this raises several difficulties from a theoretical viewpoint, it does not change the optimization algorithms, since those are mainly concerned with finite dimensional shape spaces, for which the structure is indeed Riemannian.

The purpose of this paper is to address both of these issues. In the first section, we briefly summarize the results of [4] on the Hamiltonian geodesic flow of the space of Sobolev diffeomorphisms of $\mathbb{R}^d$ for the right-invariant sub-Riemannian structure induced by a fixed arbitrary Hilbert space V of smooth

F. Nielsen and F. Barbaresco (Eds.): GSI 2015, LNCS 9389, pp. 159–167, 2015.
DOI: 10.1007/978-3-319-25040-3_18

enough vector fields. In the second part of this paper, we define abstract shape spaces in $\mathbb{R}^d$ as Banach manifolds on which the group of diffeomorphisms of $\mathbb{R}^d$ acts in a way that is compatible with its particular topological group structure. We then define the sub-Riemannian structure induced on $\mathcal{S}$ by this action and by V, and see that it admits a global Hamiltonian geodesic flow.

2 Sub-Riemannian Structures on Groups of Diffeomorphisms

The purpose of this section is to give a brief summary of the results of [4].

Fix $d \in \mathbb{N}$. For an integer $s > d/2+1$, let $\mathcal{D}^s(\mathbb{R}^d) = e + H^s(\mathbb{R}^d, \mathbb{R}^d) \cap \mathrm{Diff}(\mathbb{R}^d)$ be the connected component of $e = \mathrm{Id}_M$ in the space of diffeomorphisms of class H^s. It is an open subset of the affine Hilbert space $e + H^s(\mathbb{R}^d, \mathbb{R}^d)$, and therefore a Hilbert manifold. It is also a group for the composition $(\varphi, \psi) \mapsto \varphi \circ \psi$. This group law satisfies the following properties:

1. **Continuity:** $(\varphi, \psi) \mapsto \varphi \circ \psi$ is continuous.
2. **Smoothness on the left:** For every $\psi \in \mathcal{D}^s(\mathbb{R}^d)$, the mapping $R_\psi : \varphi \mapsto \varphi \circ \psi$ is smooth.
3. **Smoothness on the right:** For every $k \in \mathbb{N} \setminus \{0\}$, the mappings
$$\begin{aligned} \mathcal{D}^{s+k}(\mathbb{R}^d) \times \mathcal{D}^s(\mathbb{R}^d) &\longrightarrow \mathcal{D}^s(\mathbb{R}^d) \quad & H^{s+k}(\mathbb{R}^d, \mathbb{R}^d) \times \mathcal{D}^s(\mathbb{R}^d) &\longrightarrow H^s(\mathbb{R}^d, \mathbb{R}^d) \\ (\varphi, \psi) &\longmapsto \varphi \circ \psi & (X, \psi) &\longmapsto X \circ \psi \end{aligned} \tag{1}$$
are of class $\mathcal{C}^k$.
4. **Regularity:** For any $\varphi_0 \in \mathcal{D}^s(\mathbb{R}^d)$ and $X(\cdot) \in L^2(0,1; H^s(\mathbb{R}^d, \mathbb{R}^d))$, there is a unique curve $\varphi(\cdot) \in H^1(0,1; \mathcal{D}^s(\mathbb{R}^d))$ such that $\varphi(0) = \varphi_0$ and $\dot{\varphi}(t) = X(t) \circ \varphi(t)$ almost everywhere on $[0,1]$.

See [9,12,15,16] for more on this structure.

Sub-Riemannian structures on $\mathcal{D}^s(\mathbb{R}^d)$.

Definition 1. *We define a strong right-invariant structure on $\mathcal{D}^s(\mathbb{R}^d)$ as follows: fix V an arbitrary Hilbert space of vector fields with Hilbert product $\langle \cdot, \cdot \rangle_V$ and norm $\| \cdot \|_V$ and continuous inclusion in $H^{s+k}(\mathbb{R}^d, \mathbb{R}^d)$, $k \in \mathbb{N} \setminus \{0\}$. The* ***sub-Riemannian structure*** *induced by V on $\mathcal{D}^s(\mathbb{R}^d)$ is the one for which horizontal curves satisfy $\dot{\varphi}(t) = X(t) \circ \varphi(t)$, with $X \in L^2(0,1; V)$, and have total action $A(\varphi) = A(X) = \frac{1}{2} \int_0^1 \|X(t)\|_V^2 dt$.*

Define $K_V : V^* \to V$ the canonical isometry: for $P \in V^*$, $P = \langle K_V P, \cdot \rangle_V$.

Such a space V admits a reproducing kernel: a matrix-valued mapping $(x, y) \mapsto K(x, y)$ defined on $\mathbb{R}^d \times \mathbb{R}^d$ such that, for any $P \in H^s(\mathbb{R}^d, \mathbb{R}^d)^* = H^{-s}(\mathbb{R}^d, \mathbb{R}^{d*})$, the vector field $K_V P$ is given by convolution (in the distributional sense) of P with K:

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

Geodesics on $\mathcal{D}^s(\mathbb{R}^d)$. We keep the framework and notations used in the previous section, with $V \hookrightarrow H^{s+k}(\mathbb{R}^d, \mathbb{R}^d)$ and $k \geqslant 1$. Define the *endpoint map* from e by $\mathrm{end} : L^2(0,1;V) \to \mathcal{D}^s(\mathbb{R}^d)$ such that $\mathrm{end}(X) = \varphi^X(1)$. It is of class $\mathcal{C}^k$. A *geodesic* $\varphi^X(\cdot)$ from e is a critical point of the action $A(X(\cdot))$ among all horizontal curves $\varphi^Y(\cdot)$ from e with the same endpoint $\varphi^Y(1) = \varphi_1$. In other words, for every $\mathcal{C}^1$ variation $a \in (-\varepsilon, \varepsilon) \mapsto X_a(\cdot) \in L^2(0,1;V)$ such that $\mathrm{end}(X_a) = \varphi_1$, we have $\partial_a(A(X_a(\cdot))_{|a=0} = 0$.

Normal geodesics. It is easy to see that for any such curve, the couple of linear maps

$$(\mathrm{d}A(X(\cdot)), \mathrm{d}\,\mathrm{end}(X(\cdot))) : L^2(0,1;V) \to \mathbb{R} \times T_{\varphi_1}\mathcal{D}^s(\mathbb{R}^d)$$

is **not** onto. A sufficient condition for this to be true is that there exists $P_{\varphi_1} \in T^*_{\varphi_1}\mathcal{D}^s(\mathbb{R}^d) = H^{-s}(\mathbb{R}^d, \mathbb{R}^{d*})$ such that $(\mathrm{d}\,\mathrm{end}(X(\cdot)))^*.P_{\varphi_1} = \mathrm{d}A(X(\cdot))$. If such a P_1 exists, the curve induced by X is called a *normal geodesic*. This is not the only possibility [1,3,14], but it is the one we will focus on, as it is enough for inexact matching problems.

Define the normal Hamiltonian $H : T^*\mathcal{D}^s(\mathbb{R}^d) \to \mathbb{R}$ by

$$H(\varphi, P) = \frac{1}{2}P(dR_\varphi K_V dR^*_\varphi P) = \frac{1}{2}\iint_{\mathbb{R}^d \times \mathbb{R}^d} P(x)K(\varphi(x), \varphi(y))P(y)\mathrm{d}y\mathrm{d}x,$$

with K_V the isometry $V^* \to V$ and $dR_\varphi(\cdot) = \cdot \circ \varphi$ on $H^s(\mathbb{R}^d, \mathbb{R}^d)$. H is of class at least $\mathcal{C}^k$. Its symplectic gradient $\nabla^\omega H(\varphi, P) = (\partial_P H(\varphi, P), -\partial_\varphi H(\varphi, P))$ is of class $\mathcal{C}^{k-1}$.

We have the following theorem.

Theorem 1. *If $k \geqslant 1$, $\varphi(\cdot)$ is a geodesic if and only if it is the projection to $\mathcal{D}^s(\mathbb{R}^d)$ of an integral curve of $\nabla^\omega H(\varphi, P)$. In this case, the corresponding $P(\cdot)$ is the associated* ***normal covector****.*

If $k \geqslant 2$, then the symplectic gradient of the Hamiltonian admits a well-defined global flow of class $\mathcal{C}^{k-1}$, called the Hamiltonian geodesic flow. In other words, for every $(\varphi_0, P_0) \in T^*\mathcal{D}^s(\mathbb{R}^d)$, there is a unique solution $(\varphi(\cdot), P(\cdot)) : \mathbb{R} \to T^*\mathcal{D}^s(\mathbb{R}^d)$ to the Cauchy problem $(\varphi(0), P(0)) = (\varphi_0, P_0)$, $(\dot\varphi(t), \dot P(t)) = (\partial_P H(\varphi(t), P(t)), -\partial_\varphi H(\varphi(t), P(t)))$ a.e. $t \in [0,1]$. Moreover, any subarc of this solution projects to a normal geodesic on $\mathcal{D}^s(\mathbb{R}^d)$ and, conversely, any normal geodesic is the projection of such a solution.

Momentum formulation. We define the *momentum map* $\mu : T^*\mathcal{D}^s(\mathbb{R}^d) \to H^s(\mathbb{R}^d)^* = H^{-s}(\mathbb{R}^{d^*})$ by $\mu(\varphi, P) = \mathrm{d}R^*_\varphi P$.

Proposition 1. *We assume that $k \geqslant 1$. Then a horizontal curve $\varphi(\cdot) \in H^1(0,1;\mathcal{D}^s(\mathbb{R}^d))$, flow of $X(\cdot) \in L^2(0,1;V)$, is a normal geodesic with normal covector $P(\cdot)$ if and only if the corresponding momentum $\mu(t) = \mu(\varphi(t), P(t))$ along the curve satisfies, for almost every time t, $\dot\mu(t) = \mathrm{ad}^*_{X(t)}\mu(t) = -\mathcal{L}_{X(t)}\mu(t)$. Here, $\mathrm{ad}_X : H^{s+1}(\mathbb{R}^d, \mathbb{R}^d) \to H^s(\mathbb{R}^d, \mathbb{R}^d)$, with*

$\mathrm{ad}_X Y = [X, Y]$, *and* $\mathcal{L}_X$ *the Lie derivative with respect to* X. *In particular, this equation integrates as*

$$\mu(t) = \varphi(t)_* \mu(0),$$

for every $t \in [0, 1]$ *in the sense of distributions.*

We recognize the usual EPDiff equations [6,7,13]. See [2,4] for further results on such sub-Riemannian structures on $\mathcal{D}^s(\mathbb{R}^d)$, and [3,11] for more general infinite dimensional sub-Riemannian structures.

3 Shape Spaces

3.1 Definition

Throughout the section, fix a positive integer d and let s_0 be the smallest integer such that $s_0 > d/2$. A shape space in $\mathbb{R}^d$ is a Banach manifold acted upon by $\mathcal{D}^s(\mathbb{R}^d)$ for some s in a way that is compatible with its particular topological group structure. The following definition is adapted from that of [5].

Definition 2. *Let* $\mathcal{S}$ *be a Banach manifold and* $\ell \in \mathbb{N} \setminus \{0\}$, *and* $s = s_0 + \ell$. *Assume that* $\mathcal{D}^s(\mathbb{R}^d)$ *acts on* $\mathcal{S}$, *according to the action* $(\varphi, q) \mapsto \varphi \cdot q = R_q(\varphi)$. *We say that* $\mathcal{S}$ *is a shape space of order* ℓ *in* M *if the following conditions are satisfied:*

1. ***Continuity:*** $(\varphi, q) \mapsto \varphi \cdot q$ *is continuous.*
2. ***Smoothness on the left:*** *For every* $q \in \mathcal{S}$, *the mapping* $R_q : \varphi \mapsto \varphi \cdot q$ *is smooth. Its differential at* e *is denoted* ξ_q, *and is called the* ***infinitesimal action*** *of* $H^s(\mathbb{R}^d, \mathbb{R}^d)$.
3. ***Smoothness on the right:*** *For every* $k \in \mathbb{N}$, *the mappings*

$$\begin{aligned} R_q : \mathcal{D}^{s+k}(\mathbb{R}^d) \times \mathcal{S} &\longrightarrow \mathcal{S} \\ (\varphi, q) &\longmapsto \varphi \cdot q \end{aligned} \qquad \text{and} \qquad \begin{aligned} \xi : H^{s+k}(\mathbb{R}^d, \mathbb{R}^d) \times \mathcal{S} &\longrightarrow T\mathcal{S} \\ (X, q) &\longmapsto \xi_q X \end{aligned} \tag{2}$$

   are of class $\mathcal{C}^k$.
4. ***Regularity:*** *For every* $X(\cdot) \in L^2(0, 1; H^s(\mathbb{R}^d, \mathbb{R}^d))$ *and* $q_0 \in \mathcal{S}$, *there exists a unique curve* $q(\cdot) = q^X(\cdot) \in H^1(0, 1; \mathcal{S})$ *such that* $q^X(0) = q_0$ *and* $\dot{q}^X(t) = \xi_{q^X(t)} X(t)$ *for almost every* t *in* $[0, 1]$.

A an element q *of* $\mathcal{S}$ *is called a* ***state*** *of the shape. We say that* $q \in \mathcal{S}$ *has* ***compact support*** *if there exists a compact subset* U *of* M *such that* $R_q : \varphi \mapsto \varphi \cdot q$ *is continuous with respect to the semi-norm* $\| \cdot \|_{H^{s_0+\ell}(U,M)}$ *on* $\mathcal{D}^s(\mathbb{R}^d)$. *In other words,* q *has a compact support if* $\varphi \cdot q$ *depends only on the restriction of* φ *to a compact subset* U *of* M.

Here are some examples of some of the most widely used shape spaces:

1. $\mathcal{D}^{s_0+\ell}(\mathbb{R}^d)$ is a shape space of order ℓ for its action on itself given by composition on the left.

2. Let S be a smooth compact Riemannian manifold, and α_0 be the smallest integer greater than $\dim(S)/2$. Then $\mathcal{S} = \mathrm{Emb}^{\alpha_0+\ell}(S, \mathbb{R}^d)$, the manifold of all embeddings $q : S \to M$ of Sobolev class $H^{\alpha_0+\ell}$ are shape spaces of order ℓ. In this case, $\mathcal{D}^{s_0+\ell}(\mathbb{R}^d)$ acts on $\mathcal{S}$ by left composition $\varphi \cdot q = \varphi \circ q$, and this action satisfies all the required properties of Definition 2 (see [5] for the proof), with infinitesimal action $\xi_q X = X \circ q$. Every $q \in \mathcal{S}$ has compact support.
3. A particularly interesting case is obtained when $\dim(S) = 0$. Then $S = \{s_1, \ldots, s_n\}$ is simply a finite set. In that case, for any ℓ, the shape space $\mathcal{S} = \mathcal{C}^\ell(S, \mathbb{R}^d)$ is identified with the space of n landmarks in $\mathbb{R}^d$:

$$\mathrm{Lmk}_n(\mathbb{R}^d) = \{(x_1, \ldots, x_n) \in (\mathbb{R}^d)^n \mid x_i \neq x_j \text{ if } i \neq j\}.$$

   For every $q = (x_1, \ldots, x_n)$, the action of $\mathcal{D}^{s_0+1}(\mathbb{R}^d)$ is given by $\varphi \cdot q = (\varphi(x_1), \ldots, \varphi(x_n))$. For a vector field X of class H^{s_0+1} on M, the infinitesimal action of X at q is given by $\xi_q(X) = (X(x_1), \ldots, X(x_n))$. Spaces of landmarks are actually spaces of order 0 (see [5] for a definition).
4. Let $\mathcal{S}$ be a shape space of order $\ell \in \mathbb{N}$. Then $T\mathcal{S}$ is a shape space of order $\ell+1$, with the action of $\mathcal{D}^{s_0+\ell+1}(\mathbb{R}^d)$ on $T\mathcal{S}_1$ defined by $\varphi \cdot (q, v) = (\varphi \cdot q, \partial_q(\varphi \cdot q)(v))$.

3.2 Sub-Riemannian Structure on Shape Spaces

Let $\mathcal{S}$ be a shape space of order $\ell \geqslant 1$ in $\mathbb{R}^d$, and fix $s = s_0 + \ell$ and $k \in \mathbb{N} \setminus \{0\}$. Consider $(V, \langle \cdot, \cdot \rangle)$ an arbitrary Hilbert space of vector fields with continuous inclusion in $H^{s+k}(\mathbb{R}^d, \mathbb{R}^d)$. According to the previous section, we obtain a strong right-invariant sub-Riemannian structure induced by V on $\mathcal{D}^s(\mathbb{R}^d)$.

The framework of shape and image matching. The classical LDDMM algorithms for exact shape matching seek to minimize

$$\frac{1}{2}\int_0^1 \langle X(t), X(t) \rangle dt$$

over every $X \in L^2(0, 1; V)$ such that $\varphi^X(1) \cdot q_0 = q_1$, where the template q_0 and the target q_1 are fixed. Usually, one only wants to get "close" to the target shape, which is accomplished by minimizing

$$\frac{1}{2}\int_0^1 \langle X(t), X(t) \rangle dt + g(\varphi^X(1) \cdot q_0)$$

over every $X \in L^2(0, 1; V)$, where the endpoint constraint has been replaced with the addition of a data attachment term $g(\varphi^X(1) \cdot q_0)$ in the functional (See [5] and references therein). The function g is usually such that it reaches its minimum at q_1.

The sub-Riemannian structure. This leads us to define a sub-Riemannian structure on $\mathcal{S}$ as follows.

Definition 3. *The strong sub-Riemannian structure induced by V is the one for which horizontal curves are those that satisfy $\dot{q}(t) = \xi_{q(t)}X(t)$ for almost every $t \in [0,1]$, for some* ***control*** *$X(\cdot) \in L^2(0,1;\mathbb{R}^d)$. The curve $q(\cdot)$ is called a* ***horizontal deformation*** *of $q(0)$. Note that $q(t) = \varphi^X(t) \cdot q(0)$ for every t.*

Remark 1. If $\xi_q(V) = T_q\mathcal{S}$ for every $q \in \mathcal{S}$, this is actually a Riemannian structure. This is often the case in numerical simulations, where $\mathcal{S}$ is finite dimensional (usually a space of landmarks). However, in the general case, we *do not* obtain a Riemannian structure.

For example, for $d = 2$, take $\mathcal{S} = Emb^2(S^1,\mathbb{R}^2)$, with S^1 the unit circle, and fix the state $q = \mathrm{Id}_{S^1} \in \mathcal{S}$. If the kernel $K(x,y) = e^{-\|x-y\|^2}$ is Gaussian, all elements of V are analytic. Therefore, any $\xi_q(X) : S^1 \to \mathbb{R}^2$ with $X \in V$ is analytic, while $T_q\mathcal{S} = H^2(S^1,\mathbb{R}^2)$.

The *length* and *action* of a horizontal curve is not uniquely defined and depends on the control $X(\cdot)$. They coincide with the length and action of the flow φ^X which were defined in the previous section. The LDDMM algorithm can therefore be formulated as a search for sub-Riemannian geodesics on $\mathcal{S}$ for this structure.

Sub-Riemannian distance. Define the *sub-Riemannian distance* $d^{\mathcal{S}}_{SR}(q_0,q_1)$ as the infimum over the lengths of every horizontal system $(q(\cdot),X(\cdot))$ with $q(0) = q_0$ and $q(1) = q_1$. It is clear that $d^{\mathcal{S}}_{SR}$ is at least a semi-distance.

Sub-Riemannian geodesics on shape spaces. We assume that $\mathcal{S}$ is a shape space in $\mathbb{R}^d$ of order $\ell \geqslant 1$, and that $\mathcal{D}^s(\mathbb{R}^d)$, $s = s_0 + \ell$, is equipped with a strong right-invariant sub-Riemannian structure induced by the Hilbert space $(V,\langle\cdot,\cdot\rangle)$ of vector fields on $\mathbb{R}^d$, with continuous inclusion $V \hookrightarrow H^{s+k}(\mathbb{R}^d,\mathbb{R}^d)$ for some $k \geqslant 1$.

Geodesics. Fix an initial point q_0 and a final point q_1 in $\mathcal{S}$. The endpoint mapping from q_0 is $\mathrm{end}^{\mathcal{S}}_{q_0}(X(\cdot)) = \varphi^X(1) \cdot q_0 = R_{q_0} \circ \mathrm{end}$, where $\mathrm{end}(X(\cdot)) = \varphi^X(1) \in \mathcal{D}^s(\mathbb{R}^d)$. It is of class $\mathcal{C}^k$. A *geodesic* on $\mathcal{S}$ between the states q_0 and q_1 is a horizontal system $(q(\cdot),X(\cdot))$ joining q_0 and q_1 such that for any $\mathcal{C}^1$-family $a \mapsto X_a(\cdot) \in L^2(0,1;V)$ with $\varphi^{X_a}(1) \cdot q_0 = q_1$ for every a and $X_0 = X$, we have $\partial_a A(X_a(\cdot)) = 0$. We will, once again, focus on *normal geodesics*. A curve $q(\cdot)$ is a normal geodesic if for some control X whose flow φ^X yields $q(\cdot) = \varphi^X(\cdot) \circ q(0)$, and for some $p_1 \in T^*_{q(1)}\mathcal{S}$, we have $\mathrm{d}A(X) = \mathrm{d}\,\mathrm{end}^{\mathcal{S}}_{q_0}(X)^* p_1$.

Canonical symplectic form, symplectic gradient. We denote by ω the canonical weak symplectic form on $T^*\mathcal{S}$, given by the formula $\omega(q,p).(\delta q_1,\delta p_1;\delta q_2,\delta p_2) = \delta p_2(\delta q_1) - \delta p_1(\delta q_2)$, with $(\delta q_i,\delta p_i) \in T_{(q,p)}T^*\mathcal{S} \simeq T_q\mathcal{S} \times T^*_q\mathcal{S}$ in a canonical coordinate system (q,p) on $T^*\mathcal{S}$. A function $f : T^*\mathcal{S} \to \mathbb{R}$, differentiable at some point $(q,p) \in T^*\mathcal{S}$, admits a *symplectic gradient* at (q,p) if there exist a vector $\nabla^\omega f(q,p) \in T_{(q,p)}T^*\mathcal{S}$ such that, for every $z \in T_{(q,p)}T^*\mathcal{S}$, $df_{(q,p)}(z) = \omega(\nabla^\omega f(q,p), z)$. In this case, this symplectic gradient $\nabla^\omega f(q,p)$ is unique. Such a gradient exists if and only if $\partial_p f(q,p) \in T^{**}_q\mathcal{S}$ can be identified with a vector in $T_q\mathcal{S}$ through the canonical inclusion $T_q\mathcal{S} \hookrightarrow T^{**}_q\mathcal{S}$. In that case, we have, in canonical coordinates, $\nabla^\omega f(q,p) = (\partial_p f(q,p), -\partial_q f(q,p))$.

The normal Hamiltonian function and geodesic equation. We define the *normal Hamiltonian* of the system $H^{\mathcal{S}} : T^*\mathcal{S} \to \mathbb{R}$ by

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

where $K_q = \xi_q K_V \xi_q^* : T_q^*\mathcal{S} \to T_q\mathcal{S}$. It can usually be computed thanks to the reproducing kernel of V. This is a function of class $\mathcal{C}^k$, that admits as symplectic gradient $\nabla^\omega H^{\mathcal{S}}(q,p) = (K_q p, -\frac{1}{2}\partial_q(K_q p)^* p)$. of class $\mathcal{C}^{k-1}$ on $T^*\mathcal{S}$.

Momentum of the action and Hamiltonian flow. Recall that the *momentum map* associated to the group action of $\mathcal{D}^s(\mathbb{R}^d)$ over $\mathcal{S}$ is the mapping $\mu^{\mathcal{S}} : T^*\mathcal{S} \to H^s(\mathbb{R}^d, \mathbb{R}^d)^* = H^{-s}(\mathbb{R}^d, \mathbb{R}^{d*})$ given by $\mu^{\mathcal{S}}(q,p) = \xi_q^* p$.

Proposition 2. *A curve $(q(\cdot), p(\cdot))$ in $T^*\mathcal{S}$ satisfies the normal Hamiltonian equations $(\dot{q}(t), \dot{p}(t)) = \nabla^\omega H^{\mathcal{S}}(q(t), p(t))$ if and only if, for $\mu^{\mathcal{S}}(t) = \mu^{\mathcal{S}}(q(t), p(t))$ and $X(t) = K_V \xi_{q(t)}^* p(t)$, we have*

$$\dot{\mu}^{\mathcal{S}}(t) = \mathrm{ad}_{X(t)}^* \mu(t).$$

In particular, this is also equivalent to having $\varphi^X(\cdot)$ be a normal geodesic on $\mathcal{D}^s(\mathbb{R}^d)$ with initial covector $P(0) = \xi_{q(0)}^* p(0)$ and momentum $\mu(t) = \mu^{\mathcal{S}}(t)$ along the trajectory.

This result allows for the proof of our main result.

Theorem 2. *Assume $k \geqslant 1$. Then a horizontal curve $q(\cdot)$ with control $X(\cdot)$ is a geodesic if and only if it is the projection of an integral curve $(q(\cdot), p(\cdot))$ of $\nabla^\omega H^{\mathcal{S}}$ (that is, $(\dot{q}(t), \dot{p}(t)) = \nabla^\omega H^{\mathcal{S}}(q(t), p(t))$ for almost every t in $[0,1]$), with $X(t) = K_V \xi_{q(t)}^* p(t)$. This is also equivalent to having the flow φ^X of $X(\cdot)$ be a normal geodesic on $\mathcal{D}^s(\mathbb{R}^d)$ with momentum $\mu(t) = \mu^{\mathcal{S}}(t) = \xi_{q(t)}^* p(t)$.*

Assume $k \geqslant 2$. Then $\nabla^\omega H$ admits a ***global flow*** *on $T^*\mathcal{S}$ of class $\mathcal{C}^{k-1}$, called the* ***Hamiltonian geodesic flow****. In other words, for any initial point $(q_0, p_0) \in T^*\mathcal{S}$, there exists a unique curve $t \mapsto (q(t), p(t))$ defined on all of $\mathbb{R}$, such that $(q(0), p(0)) = (q_0, p_0)$ and, for almost every t, $(\dot{q}(t), \dot{p}(t)) = \nabla^\omega H^{\mathcal{S}}(q(t), p(t))$. We say that $p(\cdot)$ is the normal covector along the trajectoy.*

Combining those results, we see that solutions of the normal Hamiltonian equations on $\mathcal{S}$ are exactly those curves that come from normal geodesics on $\mathcal{D}^s(\mathbb{R}^d)$ with initial momentum of the form $\xi_{q_0}^* p_0$. In particular, for $k \geqslant 2$, the completeness of the normal geodesic flow on $T^*\mathcal{D}^s(\mathbb{R}^d)$ implies that $\nabla^\omega H^{\mathcal{S}}$ is a complete vector field on $T^*\mathcal{S}$.

On inexact matching. It should be emphasized, again, that other geodesics may also exist [4]. However, when performing LDDMM methods and algorithms for inexact matching, one aims to minimize over $L^2(0,1;V)$ functionals of the form

$$J(X(\cdot)) = A(X(\cdot)) + g(q^X(1)) = A(X(\cdot)) + g \circ \mathrm{end}_{q_0}^{\mathcal{S}}(X(\cdot)).$$

In this case, $X(\cdot)$ is a critical point if and only if $dA(X) = -\mathrm{d}\,\mathrm{end}_{q_0}^{\mathcal{S}}(X)^* dg(q^X(1))$. The trajectory induced by such a critical point X is therefore automatically a normal geodesic, whose covector satisfies $p(1) = -dg(q^X(1))$ (or, equivalently, whose momentum satisfies $\mu(1) = -\xi_{q(1)}^* dg(q^X(1)))$. This means that one needs only consider normal geodesics when looking for minimizers of J. Consequently, the search for minimizing trajectories can be reduced to the minimization of

$$\frac{1}{2}\int_0^1 p(t)(K_{q(t)}p(t))dt + g(q(1))$$

among all solutions of the control system $\dot{q}(t) = K_{q(t)}p(t)$, where $p(\cdot)$ is any covector along $q(\cdot)$ and is L^2 in time. This leads to the usual LDDMM methods.

This reduction is very useful in practical applications and numerical simulations, since, when $\mathcal{S}$ is finite dimensional, we obtain a finite dimensional control system, for which many optimization methods are available. See [5] for algorithms to minimize such a functional in the abstract framework of shape spaces in $\mathbb{R}^d$.

The case of images. Images are elements I of the functional space $L^2(\mathbb{R}^d, \mathbb{R})$. They are acted upon by $\mathcal{D}^s(\mathbb{R}^d)$ through $(\varphi, I) \mapsto I \circ \varphi^{-1}$. For a fixed template I_0 and target I_1, one aims to minimize a functional of the form

$$J(X(\cdot)) = A(X(\cdot)) + g\left(I(1)^{-1}\right),$$

with $g(I) = c\|I - I_1\|_{L^2}^2$, $c > 0$ fixed, and $I(t) = I_0 \circ \varphi(t)^{-1}$.

However, the action $(\varphi, I) \mapsto I \circ \varphi^{-1}$ *does not* make $L^2(\mathbb{R}^d, \mathbb{R})$ into a shape space, because it is not continuous. To circumvent this difficulty and still apply the framework developed in this paper, one can simply work on the shape space $\mathcal{D}^s(\mathbb{R}^d)$ itself. In this case, as long as the template I_0 belongs to $\mathcal{C}^1(\mathbb{R}^d, \mathbb{R})$, we can easily check that $\varphi \mapsto g\left(I_0 \circ \varphi^{-1}\right)$ is of class $\mathcal{C}^1$, which implies, according to the results of this section and a quick computation, that minimizers of J are those vector fields whose flow are normal geodesics with final momentum given by

$$\mu(1) = (I_1 - I(1))\, dI(1) \in L^2(\mathbb{R}^d, \mathbb{R}^{d*}).$$

References

1. Agrachev, A.A., Sachkov, Y.L.: Control Theory from the Geometric Viewpoint. Encyclopaedia of Mathematical Sciences, vol. 87. Springer, Heidelberg (2004)
2. Agrachev, A.A., Caponigro, M.: Controllability on the group of diffeomorphisms. Ann. Inst. H. Poincaré Anal. Non Linéaire **26**(6), 2503–2509 (2009)
3. Arguillère, S.: Infinite dimensional sub-Riemannian geometry and applications to shape analysis. Ph.D. thesis (2014)
4. Arguillère, S., Trélat, E.: Sub-Riemannian structures on groups of diffeomorphisms. Preprint http://arxiv.org/abs/1409.8378 (2014)

5. Arguillère, S., Trélat, E., Trouvé, A., Younes, L.: Shape deformation analysis from the optimal control viewpoint. J. Math. Pures et Appliquées (2014). arxiv.org/abs/1401.0661
6. Arnold, V.: Sur la géométrie différentielle des groupes de Lie de dimension infinie et ses applications à l'hydrodynamique des fluides parfaits. Ann. Inst, Fourier (Grenoble), 16(1), 319–361 (1966)
7. Bauer, M., Bruveris, M., Harms, P., Michor, P.W.: Geodesic distance for right invariant sobolev metrics of fractional order on the diffeomorphism group. Ann. Glob. Anal. Geom. **44**(1), 5–21 (2013)
8. Dupuis, P., Grenander, U., Miller, M.I.: Variational problems on flows of diffeomorphisms for image matching. Quart. Appl. Math. **56**(3), 587–600 (1998)
9. Ebin, D.G., Marsden, J.: Groups of diffeomorphisms and the motion of an incompressible fluid. Ann. Math. **2**(92), 102–163 (1970)
10. Grenander, U., Miller, M.I.: Computational anatomy: an emerging discipline. Quart. Appl. Math. **56**(4), 617–694 (1998). Current and future challenges in the applications of mathematics, Providence, RI (1997)
11. Grong, E., Markina, I., Vasil'ev, A.: Sub-Riemannian geometry on infinite-dimensional manifolds. Preprint arxiv.org/abs/1201.2251 (2012)
12. Kriegl, A., Michor, P.W.: The Convenient Setting of Global Analysis. Mathematical Surveys and Monographs, vol. 53. American Mathematical Society, Providence (1997)
13. Michor, P.W., Mumford, D.: An overview of the Riemannian metrics on spaces of curves using the Hamiltonian approach. Appl. Comput. Harmon. Anal. **23**(1), 74–113 (2007)
14. Montgomery, R.: A Tour of Subriemannian Geometries, Their Geodesics and Applications. Mathematical Surveys and Monographs, vol. 91. American Mathematical Society, Providence (2002)
15. Omori, H.: Infinite Dimensional Lie Transformation Groups. Lecture Notes in Mathematics, vol. 427. Springer, Berlin (1974)
16. Schmid, R.: Infinite dimensional Lie groups with applications to mathematical physics. J. Geom. Symmetry Phys. **1**, 54–120 (2004)
17. Trouvé, A.: Action de groupe de dimension infinie et reconnaissance de formes. C. R. Acad. Sci. Paris Sér. I Math. **321**(8), 1031–1034 (1995)
18. Trouvé, A.: Diffeomorphism groups and pattern matching in image analysis. Int. J. Comput. Vis. **37**(1), 17 (2005)
19. Trouvé, A., Younes, L.: Local geometry of deformable templates. SIAM J. Math. Anal. **37**(1), 17–59 (2005). (Electronic)
20. Trouvé, A., Younes, L.: Shape spaces. In: Scherzer, O. (ed.) Handbook of Mathematical Methods in Imaging, pp. 1309–1362. Springer, New York (2011)
21. Younes, L.: Shapes and Diffeomorphisms. Applied Mathematical Sciences, vol. 171. Springer, Berlin (2010)