Shapes analysis for time series.

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Abstract

In this paper, we propose an unsupervised representation learning method (URL) for time series by giving a special attention to their *shapes* for studying inter-variability in biomedical applications. In particular, the method can handle *irregularly sampled* time series having *different sizes*. This work belongs to the shape analysis litterature: we extend Large Deformation Diffeomorphic Metric Mapping (LDDMM) to the case of time series data by applying deformations to their graph. However, the method is not a simple application of LDDMM since time series graph have more structure than 1D curves. Indeed, a graph time series transformed by a general diffeomorphism is not always a graph time series. We solve this issue by establishing a representation theorem on time series graph and derive its consequences on LDDMM. This work is at the crossroad of URL for time series and shape analysis; we hope it will benefit to both communities. We demonstrate the advantages of our representation compared to existing methods using synthetic data and real-world examples, motivated by applications in medicine.

1 Introduction

Our goal is to analyze the inter-individual variability of a time series dataset, which is of prime interest in medicine and biology [42, 3, 17]. More specifically, we aim to find an unsupervised features representation method which encode the specificity of an individual compared to another. In physiology, studying the different *shapes* in a time series related to biological phenomena and their variations according to individual or pathology is common. However, a *shape* has no clear definition; it is more an intuitive way to speak about the silhouette of a pattern in a time series. In this paper, we refer to as the shape of a time series, the graph of this signal.

Although a community structure with representatives can be learned in an unsupervised way [40, 29] using contrastive loss [16, 39, 29] or similarity measures [1, 17, 35, 44], studying the inter-individual variability of shapes within a cluster [33, 38] is still an open problem in URL.

First, we propose not to see time series through their curve $\{s_t : \ t \in \mathsf{I}\}$, but through their graph $\mathsf{G}(s) = \{(t, s(t)) : \ t \in \mathsf{I}\}$. Then, building on the shape analysis litterature [4, 41], we follow the Large Deformation Diffeomorphic Metric Mapping (LDDMM) framework [4, 41] to analyze these graphs. The idea is to represent each element $(\mathsf{G}(s^j))_{j\in[N]}$ of the dataset as the transformation of a reference graph $\mathsf{G}(\mathbf{s}_0)$ by a diffeomorphism. Then, the diffeomorphism is learned by integrating an ordinary differential equation parameterized by a Reproducing Kernel Hilbert Space (RKHS). The parameters $(\alpha_j)_{j\in[N]}$ encoding the diffemorphisms $(\phi_j)_{j\in[N]}$ yield the representation features of the graphs $(\mathsf{G}(s^j))_{j\in[N]}$. Finally, these features encoding the shapes can feed any statistical or machine learning model as in URL.

However, a graph time series transformation by a general diffeomorphism is not always a graph time series, see e.g. Figure 1, thus a graph time series is more than a simple 1D curve [19]. Our contributions arise from this observation. We solve this issue by specifying the class of diffeomorphisms to

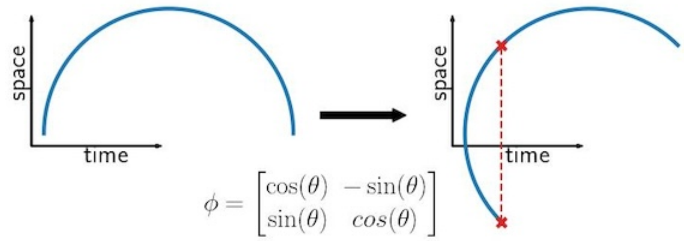

Figure 1: A time series' graph $\mathsf{G} = \{(t, s(t)) : \ t \in \mathsf{I}\}$ can lose its structure after applying a general diffeomorphism $\phi.\mathsf{G}$: a time value can be related to two values on the space axis.

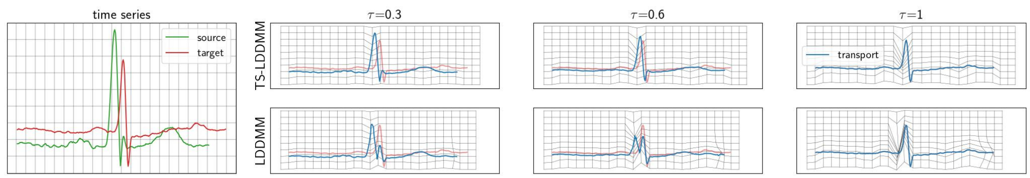

Figure 2: LDDMM and TS-LDDMM are applied to ECG data. We observe that LDDMM, using a general Gaussian kernel, does not learn the time translation of the first spike but changes the space values, i.e., one spike disappears before emerging at a translated position. At the same time, TS-LDDMM handles the time change in the shape. This difference of *deformations* implies differences in features *representations*.

consider and showing how to learn them. This change is fruitful in representing time transformation as illustrated in Figure 2. In particular, the method can handle *irregularly sampled* time series having *different sizes*.

Our contributions can be summarized as follows:

- We propose an unsupervised method (TS-LDDMM) to analyze inter-individual variability of shapes in a time series dataset. We especially motivate our extension of LDDMM to time series by introducing a theoretical framework with a representation theorem for time series graph (Theorem 1) and kernels related to their structure (Lemma 1).

- We demonstrate the identifiability of the model by estimating the true generating parameter of synthetic data, and we highlight the sensitivity of our method with respect to its hyperparameters, also providing guidelines for tuning. We highlight the *interpretability* of TS-LDDMM for studying the inter-individual variability in a clinical dataset. We illustrate the quantitative interest of the representation on classification tasks on real shape-based datasets.

2 Related Works

The main idea is to represent these different objects in a complete Riemannian manifold $(\mathcal{M}, \mathbf{g})$ with a metric $\mathbf{g}$ adapted to the geometry of the problem [30]. Then, any set of points in $\mathcal{M}$ can be represented as points in the tangent space of their Frechet mean $\mathbf{m}_0$ [34, 26] by considering their logarithms.

In this regard, this work is not an application of LDDMM to 1D curves [19]. Compared to Normalizing Flows [36, 25] or Continuous Normalizing Flows [9, 20, 37] for diffeomorphisms learning, the number of hyperparameters to tune is minimal, and the related optimization problem is well-posed.

3 Notations

We denote by integer ranges by $[k : l] = \{k, \dots, l\} \subset \mathcal{P}(\mathbb{Z})$ and $[l] = [1 : l]$ with $k, l \in \mathbb{N}$, by $\mathrm{C}^m(\mathsf{I}, \mathsf{E})$ the set of m-times continously differentiable function defined on an open set U to a normed vector space E, by $||u||_\infty = \inf_{x \in \mathsf{U}} |u(x)|$ for any bounded function $u : \mathsf{U} \to \mathsf{E}$, and by $\mathbb{N}_{>0}$ is the set of positive integers.

4 Background on LDDMM

In this part, there is no novelty, we simply expose how to learn the diffeomorphisms $(\phi_j)_{j \in [N]}$ using LDDMM, initially introduced in [4]. In a nutshell, for any $j \in [N]$, ϕ_j corresponds to a differential flow related to a learnable velocity field belonging to a well-chosen Reproducing Kernel Hilbert Space (RKHS).

In the next section, the time series are going to be represented by diffeomorphism parameters $(\alpha_j)_{j \in [N]}$. That's why LDDMM is chosen since it offers a parametrization for diffemorphisms which is sparse and interpretable, two features particularly relevant in the biomedical context.

The basic problem that we consider in this section is the following. Given a set of targets $\mathbf{y} = (y_i)_{i \in [T_2]}$ in $\mathbb{R}^{d'}$[1], a set of starting points $\mathbf{x} = (x_i)_{i \in [T_1]}$ in $\mathbb{R}^{d'}$, we aim to find a diffeomorphism ϕ such that the finite set of points $\mathbf{y}$ is similar in a certain sense to the set of finite sets of transformed points $\phi \cdot \mathbf{x} = (\phi(x_i))_{i \in [T_1]}$. The function ϕ is occasionally referred to as a *deformation*. In general, these sets $\mathbf{x}, \mathbf{y}$ are meshes of continous objects, e.g surfaces, curves, images and so on.

Representing diffeomorpshims as deformations. Such *deformations* ϕ are constructed via differential flow equations, for any $x_0 \in \mathbb{R}^{d'}$ and $\tau \in [0, 1]$:

$$\frac{\mathrm{d}X(\tau)}{\mathrm{d}\tau} = v_\tau(X(\tau)), \quad X(0) = x_0 \;, \phi^v_\tau(x_0) = X(\tau), \quad \phi^v = \phi^v_1 \;, \tag{1}$$

where the velocity field is $v : \tau \in [0, 1] \mapsto v_\tau \in \mathsf{V}$ and V is a Hilbert space of continuously differentiable function on $\mathbb{R}^{d'}$. If $||\,\mathrm{d}u||_\infty + ||u||_\infty \leq ||u||_{\mathsf{V}}$ for any $u \in \mathsf{V}$ and $v \in \mathrm{L}^2([0, 1], \mathsf{V}) = \{v \in \mathrm{C}^0([0, 1], \mathsf{V}) : \int_0^1 ||v_\tau||^2_{\mathsf{V}} \,\mathrm{d}\tau < \infty\}$, by [18, Theorem 5] ϕ^v exists and belongs to $\mathcal{D}(\mathbb{R}^{d'})$, where we denote by $\mathcal{D}(\mathsf{O})$ the set of diffeomorpshim defined on an open set O to O. Therefore, for any choice of v, ϕ^v defines a valid deformation. This offers a general recipe to construct diffeomorphism given a functional space V.

With this in mind, the velocity field v fitting the data can be estimated by minimizing $v \in \mathrm{L}^2([0, 1], \mathsf{V}) \mapsto \mathscr{L}(\phi^v.\mathbf{x}, \mathbf{y})$, where $\mathscr{L}$ is an appropriate loss function. However, two computational challenges arise. First, this optimization problem is ill-posed, and a penalty term is needed to obtain a unique solution. In addition, we have to find a parametric family $\mathsf{V}_\Theta \subset \mathrm{L}^2([0, 1], \mathsf{V})$, parameterized by Θ, which allows us to solve this minimization problem efficiently.

It has been proposed in [30] to interpret V as a tangent space relative to the space of deformations. Following this geometric point of view, geodesics can be constructed on the space of deformations by using the norm of V. More precisely, on the group of diffeomorphisms $\mathsf{H} = \{\phi^v : \; v \in \mathrm{L}^2([0, 1], \mathsf{V})\}$, the following squared norm can be defined

$$\mathscr{R}^2 : g \in \mathsf{H} \mapsto \inf_{v \in \mathrm{L}^2([0,1], \mathsf{V}) :\, g = \phi^v} \int_0^1 ||v_\tau||^2_{\mathsf{V}} \,\mathrm{d}\tau$$

as the minimal "energy" needed to perform the deformation g. By [18, Theorem 6], there exists $v^* \in \mathrm{L}^2([0, 1], \mathsf{V})$ such that the previous infimum is a minimum in v^* such that $(\phi^{v^*}_\tau)_{\tau \in [0,1]}$ can be understood as the geodesic between the identity function and g. However, given a diffeomorphism g, computing $\mathscr{R}(g)$ is intractable in most cases. To circumvent this issue, another characterization of geodesics can be considered. As in Riemannian geometry, instead of defining geodesics from their starting and end points, it is possible to define them from their starting point (here, the identity function) and an initial velocity $v_0 \in \mathsf{V}$. To CHANGE In other words, an Exponential map on deformations is wanted: given $v_0 \in \mathsf{V}$, it has been suggested to generate diffeomorphisms as $\varphi^{\{v_0\}} = \phi^v$ with By setting V as an RKHS, the geodesic shooting problem (**??**) has a unique solution and becomes tractable, as described in the next section.

[1] Note that we denote by $d' \in \mathbb{N}$ the ambient space

Discrete parametrization of diffeomorpshim. In this part, V is chosen as an RKHS [5] generated by a smooth kernel K (e.g., Gaussian). We follow [13] and define a discrete parameterization of the velocity fields to perform geodesics shooting (**??**). The initial velocity field v_0 is chosen as a finite linear combination of the RKHS basis vector fields, $\mathbf{n}_0$ control points $\mathsf{X}_0 = (x_{k,0})_{k\in[\mathbf{n}_0]} \in (\mathbb{R}^{d'})^{\mathbf{n}_0}$ and momentum vectors $\alpha_0 = (\alpha_{k,0})_{k\in[\mathbf{n}_0]} \in (\mathbb{R}^{d'})^{\mathbf{n}_0}$ are defined such that for any $x \in \mathbb{R}^{d'}$,

$$v_0\left(\alpha_0, \mathsf{X}_0\right)(x) = \sum_{k=1}^{\mathbf{n}_0} K(x, x_{k,0})\alpha_{k,0} \ . \tag{2}$$

In our applications, the control points $(x_{k,0})_{k\in[\mathbf{n}_0]}$ can be understood as the discretized graph $(t_k, \mathbf{s}_0(t_k))_{k\in[\mathbf{n}_0]}$ of a starting time series $\mathbf{s}_0$. With this parametrization of v_0, **(author?)** [30] show that the velocity field v of the solution of (**??**) keeps the same structure along time, such that for any $x \in \mathbb{R}^{d'}$ and $\tau \in [0, 1]$,

$$v_\tau(x) = \sum_{k=1}^{\mathbf{n}_0} K(x, x_k(\tau))\alpha_k(\tau) \ ,$$

$$\begin{cases} \dfrac{\mathrm{d}x_k(\tau)}{\mathrm{d}\tau} = v_\tau(x_k(\tau)) \ , \quad \dfrac{\mathrm{d}\alpha_k(\tau)}{\mathrm{d}\tau} = -\displaystyle\sum_{k=1}^{\mathbf{n}_0} \mathrm{d}_{x_k(\tau)}K(x_k(\tau), x_l(\tau))\alpha_l(\tau)^\top\alpha_k(\tau) \\ \alpha_k(0) = \alpha_{k,0}, \quad x_k(0) = x_{k,0} \ , k \in [\mathbf{n}_0] \end{cases} \tag{3}$$

These equations are derived from the hamiltonian $H : (\alpha_k, x_k)_{k\in[\mathbf{n}_0]} \mapsto \sum_{k,l=1}^{\mathbf{n}_0} \alpha_k^\top K(x_k, x_l)\alpha_l$, such that the velocity norm is preserved $||v_\tau||_\mathsf{V} = ||v_0||_\mathsf{V}$ for any $\tau \in [0, 1]$. By (3), the velocity field related to a geodesic v^* is fully parametrized by its initial control points and momentum $(x_{k,0}, \alpha_{k,0})_{k\in[\mathbf{n}_0]}$. Thus, given a set of targets $\mathbf{y} = (y_i)_{i\in[T_2]}$ in $\mathbb{R}^{d'}$, a set of starting points $\mathbf{x} = (x_{i,0})_{i\in[T_1]}$ in $\mathbb{R}^{d'}$, a RKHS's kernel $K : \mathbb{R}^{d'} \times \mathbb{R}^{d'} \to \mathbb{R}^{d'\times d'}$, a distance on sets $\mathscr{L}$, a numerical integration scheme of ODE and a penalty factor $\lambda > 0$, the basic geodesic shooting step minimizes the following function using a gradient descent method:

$$\mathcal{F}_{\mathbf{x},\mathbf{y}} : (\alpha_k)_{k\in[T_1]} \mapsto \mathscr{L}\left(\varphi^{\{v_0\}}.\mathbf{x}, \mathbf{y}\right) + \lambda||v_0||_\mathsf{V}^2 \ , \tag{4}$$

where v_0 is defined by (2) and $\varphi^{\{v_0\}}.\mathbf{x}$ is the result of the numerical integration of (3) using control points $\mathbf{x}$ and initial momentums $(\alpha_k)_{k\in[T_1]}$.

Relation to Continuous Normalizing Flows. One particular popular choice to address the problem of learning a diffeomorphism or a velocity field is Normalizing Flows [36, 25] (NF) or their continuous counterpart [9, 20, 37] (CNF). However, we do not rely on this class of learning algorithms for several reasons. Indeed, existing and simple normalizing flows are not suitable for the type of data that we are interested in this paper [15, 12]. In addition, they are primarily designed to have tractable Jacobian functions, while we do not require such property in our applications. Finally, the use of a differential flow solution of an ODE (1) trick is also at the basis of CNF, which then consists of learning a velocity field to address in fitting the data through a loss aiming to address the problem at hand. Nevertheless, the main difference between CNF and LDDMM lies in the parametrization of the velocity field. LDDMM uses kernels to derive closed form formula and enhance interpretability while NF and CNF take advantage of deep neural networks to scale with large dataset in high dimensions.

5 Methodology

We consider in this paper observations which consist in a population of N multivariate time series, for any $j \in [N]$, $s^j \in \mathrm{C}^1(\mathsf{I}_j, \mathbb{R}^d)$. However, we can only access a n_j-samples $\tilde{s}^j = (\tilde{s}^j_i = s^j(t^j_i))_{i\in[n_j]}$ collected at timestamps $(t^j_i)_{i\in[n_j]}$ for any $j \in [N]$. Note that **the number of samples n_j is not necessary the same accross individuals** and the timestamps can be **irregularly sampled**. We assume the time series population is globally homogeneous regarding their "shapes" even if inter-individual variability exists. Intuitively speaking, the "shape" of a time series $s : \mathsf{I} \to \mathbb{R}^d$ is encoded in its graphs $\mathsf{G}(s)$ defined as the set $\{(t, s(t)) : \ t \in \mathsf{I}\}$ and not only in its values $s(\mathsf{I}) = \{s(t) : \ t \in \mathsf{I}\}$ since the time axis is crucial. As a motivating use-case, s^j can be the time series of a heartbeat extracted from an individual's electrocardiogram (ECG), see Figure 2. The homogeneity in a resulting dataset comes from the fact that humans have similar shapes of heartbeat [43, 28].

The deformation problem. In this paper, we aim to study the inter-individual variability in the dataset by finding a relevant representation of each time series. Inspired from the framework of shape analysis [41], addressing similar problems in morphology, we suggest to represent each time series' graph $\mathsf{G}(s^j)$ as the transformation of a reference graph $\mathsf{G}(\mathbf{s}_0)$, related to a time series $\mathbf{s}_0 : \mathsf{I} \to \mathbb{R}^d$, by a diffeomorphism ϕ_j on $\mathbb{R}^{d+1}$, for any $j \in [N]$,

$$\phi_j.\mathsf{G}(\mathbf{s}_0) = \{\phi_j\left(t, \mathbf{s}_0(t)\right),\ t \in \mathsf{I}\}\ . \tag{5}$$

$\mathbf{s}_0$ will be understood as the typical representative shape common to the collection of time series $(s^j)_{j\in[N]}$. As $\mathbf{s}_0$ is supposed to be fixed, then the representation of the time series $(s^j)_{j\in[N]}$ boils down to the one of the transformation $(\phi_j)_{j\in[N]}$. We aim to learn $\mathsf{G}(\mathbf{s}_0)$ and $(\phi_j)_{j\in[N]}$.

Optimization related to (5). Defining the *discretized graphs* of the time series $(s^j)_{j\in[N]}$ and a discretization of the reference graph $\mathsf{G}(\mathbf{s}_0)$ as, for any $j \in [N]$,

$$\mathbf{y}_j = \mathsf{G}(\tilde{s}^j) = (t_i^j, \tilde{s}_i^j)_{i\in[n_j]} \in (\mathbb{R}^{d+1})^{n_j}, \quad \tilde{\mathsf{G}}_0 = (t_i^0, \tilde{s}_i^0)_{i\in[\mathbf{n}_0]} \in (\mathbb{R}^{d+1})^{\mathbf{n}_0}\ ,$$

with $\mathbf{n}_0 = \mathrm{median}((n_j)_{j\in[N]})$, the representation problem given in (5) boils down solving:

$$\mathrm{argmin}_{\tilde{\mathsf{G}}_0, (\alpha_k^j)_{k\in[\mathbf{n}_0]}^{j\in[N]}} \sum_{j=1}^{N} \mathcal{F}_{\tilde{\mathsf{G}}_0, \mathbf{y}_j}\left((\alpha_k^j)_{k\in[\mathbf{n}_0]}\right)\ , \tag{6}$$

which is carried out by a gradient descent on the control points $\tilde{\mathsf{G}}_0$ and the momentums $\alpha_j = (\alpha_k^j)_{k\in[\mathbf{n}_0]}$ for any $j \in [N]$, initialized by a dataset's time series graph of size $\mathbf{n}_0$ and by $0_{(d+1)\mathbf{n}_0}$ respectively. The optimization hyperparameter details are given in Appendix D.1. The result of the minimization $\tilde{\mathsf{G}}_0$ is then considered as the $\mathbf{n}_0$-samples of a common time series $\mathbf{s}_0$ and the momentums α_j encoding ϕ_j yields a feature vector in $\mathbb{R}^{d\mathbf{n}_0}$ of s^j for any $j \in [N]$. Finally, the vectors $(\alpha_j)_{j\in[N]}$ can be analyzed with any statistical or machine learning tools such as Principal Components Analysis (PCA), Latent Discriminant Analysis (LDA), longitudinal data analysis and so on.

Nevertheless, (6) ask to define a kernel and a loss in order to perform geodesic shooting 4, which is the purpose of the next subsection.

5.1 Application of LDDMM to time series analysis: TS-LDDMM

In this section, we present our theoretical contribution: we tailor the LDDMM framework to handle time series data. The reason is that applying a general diffeomorphism ϕ from $\mathbb{R}^{d+1}$ to a time series' graph $\mathsf{G}(s)$ can result in a set $\phi.\mathsf{G}(s)$ that does not correspond to the graph of any time series, as illustrated in the Figure 1. Thus, Time series graph have more structure than a simple 1D curve [19] and deserve their special analysis which will prove fruitful as demonstrated in 6.

To address this challenge, we need to identify an RKHS kernel $K : \mathbb{R}^{d+1} \times \mathbb{R}^{d+1} \to \mathbb{R}^{(d+1)^2}$ that generates deformations preserving the structure of the time series graph. This goal motivates us to clarify, in Theorem 1, the specific representation of diffeomorphisms we require before presenting a class of kernels that produce deformations with this representation.

Similarly, selecting a loss function on sets $\mathscr{L}$ that considers the temporal evolution in a time series' graph is crucial for meaningful comparisons with time series data. Consequently, we introduce the oriented Varifold distance.

A representation separating space and time. We prove that two time series graphs can always be linked by a time transformation composed of a space transformation. Moreover, a time series graph transformed by this kind of transformation is always a time series graph. We define $\Psi_\gamma \in \mathcal{D}(\mathbb{R}^{d+1}) : (t, x) \in \mathbb{R}^{d+1} \to (\gamma(t), x)$ for any $\gamma \in \mathcal{D}(\mathbb{R})$ and $\Phi_f : (t, x) \in \mathbb{R}^{d+1} \to (t, f(t, x))$ for any $f \in \mathrm{C}^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$. We have the following representation theorem. All proofs are given in Appendix A.

Denote by $\mathsf{G}(s) \triangleq \{(t, s(t)) :\ t \in \mathsf{I}\}$ the graph of a time series $s : \mathsf{I} \to \mathbb{R}^d$ and $\phi.\mathsf{G}(s) \triangleq \{\phi(t, s(t)) : t \in \mathsf{I}\}$ the action of $\phi \in \mathcal{D}(\mathbb{R}^{d+1})$ on $\mathsf{G}(s)$.

Theorem 1. *Let $s : \mathsf{J} \to \mathbb{R}^d$ and $\mathbf{s}_0 : \mathsf{I} \to \mathbb{R}^d$ be two continuously differentiable time seriess with I, J two intervals of $\mathbb{R}$. There exist $f \in \mathrm{C}^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$ and $\gamma \in \mathcal{D}(\mathbb{R})$ such that $\gamma(\mathsf{I}) = \mathsf{J}$ and $\Phi_f \in \mathcal{D}(\mathbb{R}^{d+1})$,*

$$\mathsf{G}(s) = \Pi_{\gamma,f}.\mathsf{G}(\mathbf{s}_0),\ \Pi_{\gamma,f} = \Psi_\gamma \circ \Phi_f .$$

Moreover, for any $\bar{f} \in \mathrm{C}^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$ and $\bar{\gamma} \in \mathcal{D}(\mathbb{R})$, there exists a continously differentiable time series $\bar{s}$ such that $\mathsf{G}(\bar{s}) = \Pi_{\bar{\gamma},\bar{f}}.\mathsf{G}(\mathbf{s}_0)$

Remark 2. *that for any $\gamma \in \mathcal{D}(\mathbb{R})$ and $s \in \mathrm{C}^0(\mathsf{I}, \mathbb{R}^d)$,*

$$\{(\gamma(t), s(t)),\ t \in \mathsf{I}\} = \{(t, s \circ \gamma^{-1}(t)) :\ t \in \gamma(\mathsf{I})\} .$$

As a result, Ψ_γ can be understood as a temporal reparametrization and Φ_f encodes the transformation about the space.

Choice for the kernel associated with the RKHS V As depicted on Figure 1-2, we can not use any kernel K to apply the previous methodology to learn deformations on time series' graphs. We describe and motivate our choice in this paragraph. Denote the one-dimensional Gaussian kernel by $K_\sigma^{(a)}(x, y) = \exp(-|x - y|^2/\sigma)$ for any $(x, y) \in (\mathbb{R}^a)^2$, $a \in \mathbb{N}$ and $\sigma > 0$. To solve the geodesic shooting problem (4) on $\mathbb{R}^{d+1}$, we consider for V the RKHS associated with the kernel defined for any $(t, x), (t', x') \in (\mathbb{R}^{d+1})^2$:

$$K_{\mathsf{G}}((t, x), (t', x')) = \begin{pmatrix} c_0 K_{\text{time}} & 0 \\ 0 & c_1 K_{\text{space}} \end{pmatrix} , \tag{7}$$
$$K_{\text{space}} = K^{(1)}_{\sigma_{T,1}}(t, t') K^{(d)}_{\sigma_x}(x, x') \mathrm{I}_d \ , K_{\text{time}} = K^{(1)}_{\sigma_{T,0}}(t, t') \ ,$$

parametrized by the widths $\sigma_{T,0}, \sigma_{T,1}, \sigma_x > 0$ and the constants $c_0, c_1 > 0$. This choice for K_{G} is motivated by the representation Theorem 1 and the following result.

Lemma 1. *If we denote by V the RKHS associated with the kernel K_{G}, then for any vector field v generated by (3) with v_0 satisfying (2), there exist $\gamma \in \mathsf{D}(\mathbb{R})$ and $f \in \mathrm{C}^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$ such that $\phi^v = \Psi_\gamma \circ \Phi_f$.*

Parler des Cauchy kernel en appndice et du choix de la loss

Remark 3. *With this choice of kernel, the features associated to the time transformation can be extracted from the momentums $(\alpha_{k,0})_{k\in[\mathbf{n}_0]} \in (\mathbb{R}^{d+1})^{\mathbf{n}_0}$ in (2) by taking the coordinates related to time. However, the features related to the space transformation are not only in the space coordinates since the related kernel K_{space} depends on time as well.*

In Appendix C, we give guidelines for selecting the hyperparameters $(\sigma_{T,0}, \sigma_{T,1}, \sigma_x, c_0, c_1)$.

Loss This section specifies the distance function $\mathscr{L}$ introduced in the loss function defined in (4).

In practice, we can only access discretized graphs of time series, $(t_i^j, \tilde{s}_i^j)_{i\in[n_j]}$ for any $j \in [N]$, that are potentially of different sizes n_j and sampled at different timestamps $(t_i^j)_{i\in[n_j]}$ for any $j \in [N]$. Usual metrics, such as the Euclidean distance, are not appealing as they make the underlying assumptions of equal size sets and the existence of a pairing between points. Distances between measures on sets (taking the empirical distribution), such as Maximum Mean Discaprency (MMD) [14, 6], alleviate those issues; however, MMD only accounts for positional information and lacks information about the time evolution between sampled points. A classical data fidelity metric from shape analysis corresponding to the distance between *oriented varifolds* associated with curves alleviates this last issue [24]. Intuitively, an oriented varifold is a measure that accounts for positional and tangential information about the underlying curves at sample points. More details and information about *oriented varifolds* can be found in Appendix B.

More precisely, given two sets $\mathsf{G}_0 = (g_i^0)_{i\in[T_0]}, \mathsf{G}_1 = (g_i^1)_{i\in[T_1]} \in (\mathbb{R}^{d+1})^{T_1}$ and a kernel[2] $k : (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2 \to \mathbb{R}$ verifying [24, Proposition 2 & 4], for any $\xi \in \{0, 1\}$ and $i \in [T_\xi - 1]$, denoting the center and length of the i^{th} segment $[g_i^\xi, g_{i+1}^\xi]$ by $c_i^\xi = (g_i^\xi + g_{i+1}^\xi)/2$, $l_i^\xi = \|g_{i+1}^\xi - g_i^\xi\|$, and

[2] $\mathbb{S}^d = \{x \in \mathbb{R}^{d+1} :\ |x| = 1\}$

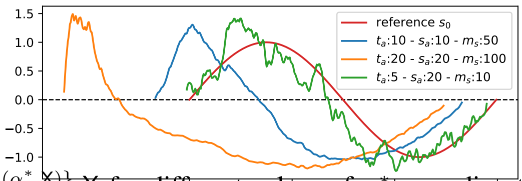

Figure 3: Plots of $\varphi^{\{v_0(\alpha^*,\mathsf{X})\}}.\mathsf{X}$ for different values of α^*, according to its sampling parameter t_a, s_a, m_s, taking $\mathsf{X} = \mathsf{G}(s_0)$ with $s_0 : k \in [300] \to \sin(2\pi k/300)$.

Table 1: Values of $\mathscr{L}(\varphi^{\{v_0(\alpha^*,\mathsf{X})\}}.\mathsf{X}, \varphi^{\{\hat{v}_0\}}.\mathsf{X})$ as α^* is sampled according to Gen(10,10,50) and $\hat{v}_0$ is estimated using K_{G} with varying parameters $\sigma_{T,1}, \sigma_x$.

$\sigma_{T,0} \backslash \sigma_x$	1	10	50	100	200	300
0.1	2e+0	3e-4	1e-5	4e-6	7e-4	4e-3
1	4e-2	1e-4	1e-5	4e-6	7e-4	4e-3
100	4e-2	2e-4	1e-5	4e-6	7e-4	4e-3

$\overrightarrow{v_i}^{\xi} = (g^{\xi}_{i+1} - g^{\xi}_i)/l^{\xi}_i$, the varifold distance between G_0 and G_1 is defined as,

$$d^2_{\mathsf{W}^*}(\mathsf{G}_0, \mathsf{G}_1) = \sum_{i,j=1}^{T_0-1} l^0_i k((c^0_i, \overrightarrow{v_i}^0), (c^0_j, \overrightarrow{v_j}^0)) l^0_j - 2 \sum_{i=1}^{T_0-1} \sum_{j=1}^{T_1-1} l^0_i k((c^0_i, \overrightarrow{v_i}^0), (c^1_j, \overrightarrow{v_j}^1)) l^1_j$$
$$+ \sum_{i,j=1}^{T_1-1} l^1_i k((c^1_i, \overrightarrow{v_i}^1), (c^1_j, \overrightarrow{v_j}^1)) l^1_j$$

In practice, we set the kernel k as the product of two anisotropic Gaussian kernels, k_{pos} and k_{dir}, such that for any $(x, \overrightarrow{u}), (y, \overrightarrow{v}) \in (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2$

$$k((x, \overrightarrow{u}), (y, \overrightarrow{v})) = k_{\text{pos}}(x, y) k_{\text{dir}}(\overrightarrow{u}, \overrightarrow{v}) \, .$$

The specific kernels $k_{\text{pos}}, k_{\text{dir}}$ that we use in our experiments are given Appendix B.1. Note that the loss kernel k has nothing to do with the velocity field kernel denoted by K_{G} or K specified in Section 5.1. Finally, we define the data fidelity loss function, $\mathscr{L}$, as $d^2_{\mathsf{W}^*}$, which is differentiable with regards to its first variable. For further readings on curves and surfaces representation as varifolds, readers can refer to [24, 8].

Parler de méthode adaptatif ici

6 Experiments

First, we show on synthetic data that the proposed representation is identifiable provided that the hyperparameters and the reference graph are wisely selected, i.e., the parameter v^*_0 generating a deformation $\varphi^{\{v^*_0\}}$ of a time series graph G can be estimated from the data $\mathsf{G}, \varphi^{\{v^*_0\}}.\mathsf{G}$ by solving the geodesic shooting problem (4). Secondly, we illustrate the qualitative interest of TS-LDDMM in studying inter-individual variability on a clinical dataset. Thirdly, we demonstrate the quantitative performance of our representation by performing classification on shape-based datasets. The method is implemented on Python using the library JAX[3]. The code was compiled on a server with NVIDIA RTX A2000 12GB GPU, Intel(R) Xeon(R) Gold 5220R CPU @ 2.20GHz, and 250 GB of RAM. The code will be available on Github.

6.1 Synthetic experiments

First, we show the model identifiability when the kernel K_G is well specified: the estimated parameter is a good approximation of the generating parameter when the generation and the estimation procedure use the same hyperparameters for the RKHS kernel K_{G}. All the hyperparameter values for generation and estimation are given in Appendix D.2. We fix the initial control points

[3] https://github.com/google/jax

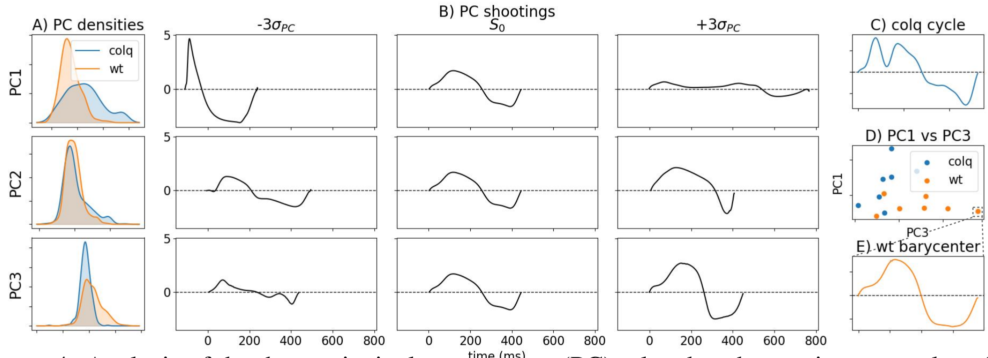

Figure 4: Analysis of the three principal components (PC) related to the respiratory cycles of the mouse before exposure. In Figure A), the densities of each genotype according to each PC are displayed. In Figure B), the deformations of the reference graph S_0 along each PC are given. In Figure D), the graph of reference S^j, also called barycenter, related to each mouse, is displayed according to their coordinates on PC1 and PC3. In Figure C) et E), illustrations of respiratory cycles related to mice coming from the **wt** and **colq** group are displayed.

as $\mathsf{X} = (x_k = (k, \sin(2\pi k/300)))_{k\in[300]}$. Given $m_s \in \mathbb{N}_{>0}$ and $t_a, s_a > 0$, we randomly generate initial momentums $\alpha^* = (\alpha_k^*)_{k\in[\mathbf{n}_0]}$ with the following sampling, called Gen(m_s, t_a, s_a): For any $k \in [\mathbf{n}_0]$, α_k' is sampled according to a Gaussian normal distribution $\mathcal{N}(0_{d+1}, I_{d+1})$. Then, $(\alpha_k')_{k\in[\mathbf{n}_0]}$ is regularized by a rolling average of size m_s, we get $\bar{\alpha}' = (\bar{\alpha}_k')_{k\in[\mathbf{n}_0]}$. Finally, we normalize $\bar{\alpha}'$ to derive α^* such that $|([\alpha_k^*]_t)_{k\in[\mathbf{n}_0]}| = t_{\text{amp}}$ and $|([\alpha_k^*]_s)_{k\in[\mathbf{n}_0]}| = s_{\text{amp}}$ for any $k \in [\mathbf{n}_0]$, denoting by $[\alpha_k^*]_t, [\alpha_k^*]_s$ the time and space coordinates of α_k^* respectively. Note that the regularizing step $(\alpha_k')_{k\in[\mathbf{n}_0]} \to \bar{\alpha}'$ is necessary to obtain realistic deformations which take into account the regularity induced by the RKHS V. Then, using $v_0(\alpha^*, \mathsf{X})$ as defined in (2) with initial momentums α^* and control points X, we apply the induced deformation $\varphi^{\{v_0\}}$ by (3) to X and obtain $\varphi^{\{v_0\}}.\mathsf{X}$. Finally, we solve (4) to recover an estimation $\hat{\alpha}$ of α^* and report the average relative error (ARE) $|v_0(\hat{\alpha}, \mathsf{X}) - v_0(\alpha^*, \mathsf{X})|_{\mathsf{V}}/|v_0(\alpha^*, \mathsf{X})|_{\mathsf{V}}$ on 50 repetitions. This procedure is performed for any $m_s, t_a, s_a \in \{10, 50, 100\} \times \{5, 10, 15, 20\}^2$. Mean, standard deviation, and maximum of the ARE on all these hyperparameters choices are respectively $\mathbf{0.10}, \mathbf{0.03}, \mathbf{0.17}$. Therefore, the estimation procedure (4) offers a good approximation of the true parameter when the kernel K_{G} is well specified. We observe that the estimation is difficult when $t_a \ll s_a$ because the time series can be very noisy as illustrated in Figure 3: this impacts the Varifold loss which is sensitive to tangents.

Secondly, we demonstrate a weak identifiability when the kernel K_{G} is misspecified: we can reconstruct the graph time series' after deformations even if the hyperparameters of K_{G} are different during the generation and the estimation. The hyperparameters of K_{G} during generation are $(c_0, c_1, \sigma_{T,0}, \sigma_{T,1}, \sigma_x) = (1, 0.1, 100, 1, 1)$ and we fix $\sigma_{T,1}, c_0, c_1 = (1, 1, 0.1)$ for K_{G} during estimation. We aim to understand the impact of $\sigma_{T,1}, \sigma_x$ on the reconstruction since they are encoding the smoothness of the transformation according to time and space.

For any choice of the hyperparameters $\sigma_{T,1}, \sigma_x \in \{1, 10, 50, 100, 200, 300\} \times \{0.1, 1, 100\}$ related to K_{G} in the estimation, we average $\mathscr{L}(\varphi^{\{v_0(\alpha^*,\mathsf{X})\}}.\mathsf{X}, \varphi^{\{\hat{v}_0\}}.\mathsf{X})$ on 50 repetitions when α^* is sampled according to Gen$(10, 10, 50)$ and $\hat{v}_0 = v_0(\hat{\alpha}, \mathsf{X})$ denoting by $\hat{\alpha}$ the result of the minimization (4). We observe in Table 1 that the reconstruction is almost perfect except in the case when $\sigma_{t,0} = 1$ during estimation, while $\sigma_{t,0} = 100$ during generation. Compared to $\sigma_{T,0}$, σ_x has nearly no impact on the reconstruction. In Appendix B.1-C, we propose guidelines to drive future hyperparameters tuning and further discussions related to $\sigma_{T,1}, c_0, c_1$.

6.2 Qualitative analysis of respiratory behavior in mice

This experiment highlights the *interpretability* of TS-LDDMM for studying the inter-individual variability in a clinical dataset. We consider a time series dataset recording the evolution of the respiratory airflow of mice exposed to an irritant molecule altering respiratory functions [32]. The dataset is divided into two groups, one composed of 7 control mice (**wt**) and the other of 7 mice (**colq**) deficient in an enzyme involved in the control of respiration. For each mouse, the respiratory

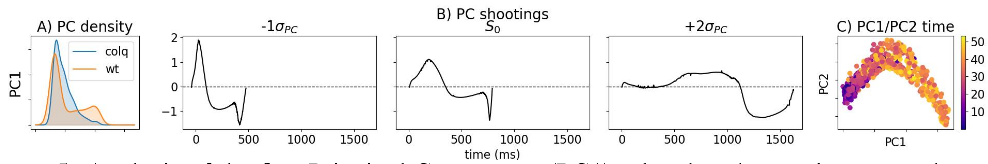

Figure 5: Analysis of the first Principal Component (PC1) related to the respiratory cycles of the mouse before and after exposure. In Figure A), the densities of each genotype according are displayed. In Figure B), the deformations of the reference graph S_0 PC1 is given. In Figure C), respiratory cycles displayed with respect to time and according to their coordinates on PC1 and PC2

airflow was recorded for 15 to 20 minutes before exposure to the irritant molecule and then for 35 to 40 minutes. A complete description of the dataset is given in the Appendix E. By comparing the shape of individual respiratory cycles (inspiration + expiration, see Figure 4-C)), we show that TS-LDDMM features can encode genotype distinctive breathing behaviors and their evolution after exposure to the irritant molecule.

We first compare breathing behaviors before exposure. Solving (6), we derive the reference respiratory cycle's graph S_0 and the TS-LDDMM features representations $(\alpha_j)_{j\in[N_1]}$ related to $N_1 = 700$ respiratory cycles extracted according to the procedure [17]. Then, we perform a kernel PCA on the initial velocity field $(v_0(\alpha_j, S_0))_{j\in[N_1]} \in \mathsf{V}^{N_1}$ defined in (2). In Figure 4, we focus on the analysis of the three Principal Components (PC).

As observable from Figure 4-B), principal components refer to different types of deformations. By interpreting Figure 4-B): Only PC1 accounts for time warping, PC2 expresses the trade-off between inspiration and expiration duration, and PC3 corresponds to a change in signal amplitude. Compared to **wt** mice, the distribution of **colq** mice TS-LDMMM feature representation along the PC1 axis has a heavy tail and the associated deformation (+3 σ_{PC}) shows an inspiration with two peaks. As illustrated in Figure 4-A), such respiratory cycles are preponderant with **colq** mice and may be caused by motor impairment due to their enzyme deficiency, [17]. In addition, the **colq** mice were smaller than the **wt** mice due to a delay in growth caused by their lack of an enzyme. This difference can be seen on PC3 since the volumes of air (area under the curve) inspired and exhaled are smaller for the smaller mice. In correlation, the distribution of **wt** mice TS-LDDMM feature representations along the PC3 axis have a heavy tail corresponding to large air volume as depicted by the deformation (+3 σ_{PC}) in Figure 4-B). Finally, Figure 4-D) shows that PC1 and PC3 capture the main differences between the two groups as their respective reference graphs S^j are located in different parts of the space.

We perform a second experiment to analyze the evolution of breathing behaviors when mice are exposed to the irritant molecule. We follow the same procedure as before. However, we take $N_2 = 1400$ with 25% (resp. 75%) before (resp. after) exposure. In Figure 5, we focus on the first principal component PC since it encodes the effect of the irritant molecule as depicted in Figure 5-C) (the exposure occurs at 20 minutes). Figure 5-B) shows that the deformation (+3 σ_{PC}) leads to longer respiratory cycles that include pauses, as observed in [17]. As well, Figure 5-A) shows that TS-LDDMM features distributions are less spread out for **colq** mice compared to **wt** mice. Indeed, the irritant molecule inhibits the action of the deficient enzyme, **wt** mice strongly react to the irritant molecule, whereas **colq** mice are better adapted due to their deficiency.

6.3 Quantitative performances of the TS-LDDMM representation in classification

Combined with a Support Vector Classifier (SVC) [22], TS-LDDMM representation can be used for classification tasks using the kernel associated with the initial velocity space V. We compare TS-LDDMM-SVC classification performances with another SVC using representation learned with T-loss [16], an unsupervised deep learning feature representation method for time series. We also include fully supervised methods in deep learning -ResNet, CNN [23]- and machine learning: Catch22 [27], Rocket [11], Dynamic Time Wrapping k-Nearest Neighbors (DTW-kNN) [31]. Methods are compared using f1-score on several shape-based UCR/UEA datasets [10, 2] introduced in Appendix F. All implementation details are given in Appendix D.4. Table 2 presents the reuslts. TS-LDDMM-SVC consistently outperforms the other unsupervised methods. It is ranked 1,3,4,3 for all methods combined, demonstrating its competitiveness as an unsupervised method on time series dataset homogeneous regarding shape.

Table 2: Classification results in f1-score (U: unsupervised, S: supervised, DL: deep learning, ML: machine learning). **x** best unsupervised method, x best supervised method.

			ArrowHead	ECG200	GunPoint	NATOPS
U		TS-LDDMM-SVC	**0.84**	**0.82**	**0.94**	**0.93**
		T-loss-SVC	0.57	0.76	0.82	0.88
		DTW-kNN	0.70	0.75	0.91	0.88
S	DL	CNN	0.70	0.79	0.85	0.96
		ResNet	0.77	0.87	0.97	0.95
	ML	Catch22	0.73	0.81	0.96	0.89
		Rocket	0.81	0.91	1.00	0.88

7 Conclusion

In this paper, we propose a feature representation method, TS-LDDMM, designed for shape comparison in homogeneous time series datasets. We show on a real dataset its ability to study, with high interpretability, the inter-individual shape variability. As an unsupervised approach, it is user-friendly and enables knowledge transfer for different supervised tasks such as classification. Although TS-LDDMM is already competitive for classification, its performances can be leveraged on more heterogeneous datasets using a hierarchical clustering extension, which is relagated for future work.

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A Proofs

Denote by $\mathsf{G}(s) \triangleq \{(t, s(t)) : t \in \mathsf{I}\}$ the graph of a time series $s : \mathsf{I} \to \mathbb{R}^d$ and $\phi.\mathsf{G}(s) \triangleq \{\phi(t, s(t)) : t \in \mathsf{I}\}$ the action of $\phi \in \mathcal{D}(\mathbb{R}^{d+1})$ on $\mathsf{G}(s)$.

Theorem 4. *Let $s : \mathsf{J} \to \mathbb{R}^d$ and $\mathbf{s}_0 : \mathsf{I} \to \mathbb{R}^d$ be two continuously differentiable time seriess with I, J two intervals of $\mathbb{R}$. There exist $f \in \mathrm{C}^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$ and $\gamma \in \mathcal{D}(\mathbb{R})$ such that $\gamma(\mathsf{I}) = \mathsf{J}$ and $\Phi_f \in \mathcal{D}(\mathbb{R}^{d+1})$,*

$$\mathsf{G}(s) = \Pi_{\gamma,f}.\mathsf{G}(\mathbf{s}_0),\ \Pi_{\gamma,f} = \Psi_\gamma \circ \Phi_f .$$

Moreover, for any $\bar{f} \in \mathrm{C}^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$ and $\bar{\gamma} \in \mathcal{D}(\mathbb{R})$, there exists a continously differentiable time series $\bar{s}$ such that $\mathsf{G}(\bar{s}) = \Pi_{\bar{\gamma},\bar{f}}.\mathsf{G}(\mathbf{s}_0)$

Proof. Let $s : \mathsf{J} \to \mathbb{R}^d$ and $\mathbf{s}_0 : \mathsf{I} \to \mathbb{R}^d$ be two continuously differentiable time seriess with $\mathsf{I} = (a, b), \mathsf{J} = (\alpha, \beta)$ two intervals of $\mathbb{R}$. By setting $\gamma : t \in \mathbb{R} \mapsto (\beta - \alpha)(t - a)/(b - a) + \alpha \in \mathbb{R}$, we have $\gamma(\mathsf{I}) = \mathsf{J}$ and $\gamma \in \mathcal{D}(\mathbb{R})$. By defining $f : (t, x) \in \mathbb{R}^{d+1} \mapsto x - \mathbf{s}_0(t) + s \circ \gamma(t)$, the map $\Phi_f \in \mathcal{D}(\mathbb{R}^{d+1})$, indeed, its inverse is $\Phi_f^{-1} : (t, x) \in \mathbb{R}^{d+1} \mapsto (t, x + \mathbf{s}_0(t) - s(t))$ and is continuously differentiable. Moreover, we have $\Pi_{\gamma,f}.\mathsf{G}(\mathbf{s}_0) = \{(\gamma(t), s \circ \gamma(t)) : t \in \mathsf{I}\} = \mathsf{G}(s)$.

Let $\bar{f} \in \mathrm{C}^0(\mathbb{R}^{d+1}, \mathbb{R}^d)$, $\bar{\gamma} \in \mathcal{D}(\mathbb{R})$ and $\mathbf{s}_0 \in \mathrm{C}^0(\mathsf{I}, \mathbb{R}^d)$ with I an interval of $\mathbb{R}$. We have :

$$\begin{aligned} \Pi_{\gamma,f}.\mathsf{G}(\mathbf{s}_0) &= \{(\gamma(t), f(t, \mathbf{s}_0(t))),\ t \in \mathsf{I}\ \} \\ &= \left\{\left(t, f\left(\gamma^{-1}(t), \mathbf{s}_0(\gamma^{-1}(t))\right)\right),\ t \in \gamma(\mathsf{I})\ \right\} . \end{aligned} \tag{8}$$

By defining $\bar{s} : t \in \gamma(\mathsf{I}) \to f\left(\gamma^{-1}(t), \mathbf{s}_0(\gamma^{-1}(t))\right)$, we have $\bar{s} \in \mathrm{C}^0(\gamma(\mathsf{I}), \mathbb{R}^d)$ by composition of continuous functions and $\mathsf{G}(\bar{s}) = \Pi_{\gamma,f}.\mathsf{G}(\mathbf{s}_0)$ by (8), which concludes the proof. □

Lemma 2. *If we denote by V the RKHS associated with the kernel K_{G}, then for any vector field v generated by* (3) *with v_0 satisfying* (2)*, there exist $\gamma \in \mathsf{D}(\mathbb{R})$ and $f \in \mathrm{C}^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$ such that $\phi^v = \Psi_\gamma \circ \Phi_f$.*

Proof. Let v be a vector field generated by (3) with v_0 satisfying (2). We remark that the first coordinate of the velocity field v_τ denoted by v_τ^{time} only depends on the time variable t for any $\tau \in [0, 1]$. Thus, when computing the first coordinate of the deformation ϕ^v, denoted by γ, we integrate (1) with v_τ replaced by v_τ^{time}, thus γ is independant of the variable x. Moreover, $\gamma \in \mathcal{D}(\mathbb{R})$ since a Gaussian kernel induced an Hilbert space V satisfying $|f|_V \leq |f|_\infty + |\,\mathrm{d}f|_\infty$ for any $f \in \mathsf{V}$ by [18, Theorem 9]. For the same reason, we have $\phi^v \in \mathcal{D}(\mathbb{R}^{d+1})$, and thus its last coordinates denoted by f belongs to $\mathrm{C}^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$, and by construction $\phi^v = \Psi_\gamma \circ \Phi_f$. □

B Oriented varifold

In this section, we introduce the *oriented varifold* associated with curves. For further readings on curves and surfaces representation as varifolds, readers can refer to [24, 8]. We associate to $\gamma \in \mathrm{C}^1((a, b), \mathbb{R}^{d+1})$ an *oriented varifold* μ_γ, i.e. a distribution on the space $\mathbb{R}^{d+1} \times \mathbb{S}^d$ defined as follows, for any smooth test function $\omega : \mathbb{R}^{d+1} \times \mathbb{S}^d \to \mathbb{R}$,

$$\mathbb{E}_{Y \sim \mu_\gamma}[\omega(Y)] = \mu_\gamma(\omega) = \int_a^b \omega\left(\gamma(t), \frac{\dot{\gamma}(t)}{|\dot{\gamma}(t)|}\right) |\dot{\gamma}(t)|\,\mathrm{d}t .$$

Denoting by W the space of smooth test function, we have that μ_γ belongs to its dual W^*. Thus, a distance on W^* is sufficient to set a distance on oriented varifolds associated to curve and thus on $\mathrm{C}^1((a, b), \mathbb{R}^{d+1})$ by the identification $\gamma \to \mu_\gamma$. Remark that in (TS-LDDMM), γ should be the parametrization of a time series' graph $\mathsf{G}(s)$, i.e. $\gamma : t \in \mathsf{I} \to (t, s(t)) \in \mathbb{R}^{d+1}$ denoting by $s : \mathsf{I} \to \mathbb{R}^d$ the time series. However, in practice, we work with discrete objects. That is why, we set W as an RKHS to use its representation theorem. More specifically [24, Proposition 2 & 4] encourages us to consider a kernel $k : (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2 \to \mathbb{R}$ such that there exist two positive and continuously differentiable kernels k_{pos} and k_{dir}, such that for any $(x, \overrightarrow{u}), (y, \overrightarrow{v}) \in (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2$

$$k((x, \overrightarrow{u}), (y, \overrightarrow{v})) = k_{\text{pos}}(x, y) k_{\text{dir}}(\overrightarrow{u}, \overrightarrow{v}) ,$$

with moreover $k_{\mathrm{dir}} > 0$ and k_{pos} which admits an RKHS $\mathsf{W}_{\mathrm{pos}}$ dense in the space of continous function on $\mathbb{R}^{d+1}$ vanishing at infinite [7].

Given such a kernel $k : (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2 \to \mathbb{R}$ verifying [24, Proposition 2 & 4], we have that for any $(x, v) \in \mathbb{R}^{d+1} \times \mathbb{S}^d$, $\delta_{(x,\overrightarrow{v})}$ belongs to W^* as a distribution and that the dual metric $\langle \cdot, \cdot \rangle_{\mathsf{W}^*}$ satisfies for any $(x_1, v_1), (x_2, v_2) \in \left(\mathbb{R}^{d+1} \times \mathbb{S}^d\right)^2$,

$$\langle \delta_{(x_1,\overrightarrow{v}_1)}, \delta_{(x_2,\overrightarrow{v}_2)} \rangle_{\mathsf{W}^*} = k((x_1, \overrightarrow{v}_1), (x_2, \overrightarrow{v}_2)) \ .$$

Thus, given two sets of triplets $X = (l_i, x_i, \overrightarrow{v}_i)_{i\in[T_0-1]} \in (\mathbb{R} \times \mathbb{R}^{d+1} \times \mathbb{S}^d)^{T_0-1}, Y = (l'_i, y_i, \overrightarrow{w}_i)_{i\in[T_1]} \in (\mathbb{R} \times \mathbb{R}^{d+1} \times \mathbb{S}^d)^{T_1-1}$ and denoting by

$$\mu_X = \sum_{i=1}^{T_0} l_i \delta_{(x_i,\overrightarrow{v}_i)}, \mu_Y = \sum_{i=1}^{T_1} l'_i \delta_{(y_i,\overrightarrow{w}_i)} \ , \tag{9}$$

we have,

$$|\mu_X - \mu_Y|^2_{\mathsf{W}^*} = \sum_{i,j=1}^{T_0-1} l_i k((x_i, \overrightarrow{v_i}), (x_i, \overrightarrow{v_i}^0)) l_j - 2 \sum_{i=1}^{T_0-1} \sum_{j=1}^{T_1-1} l_i k((x_i, \overrightarrow{v_i}), (y_i, \overrightarrow{w_i})) l'_j + \sum_{i,j=1}^{T_1-1} l'_i k((y_i, \overrightarrow{w_i}), (y_i, \overrightarrow{w_i})) l'_j \ .$$

Then, using the identification $X \to \mu_X, Y \to \mu_Y$, we can define a distance on sets of triplets as $d_{\mathsf{W}^*,3}(X, Y) = |\mu_X - \mu_Y|^2_{\mathsf{W}^*}$.

Now, we aim to discretize the oriented varifold μ_{G} related to a time series' graph $\mathsf{G}(s)$ by using a set of triplets. This is carried out by using a discretized version of $\mathsf{G}(s)$, i.e. $\tilde{\mathsf{G}} = (g_i = (t_i, s(t_i)))_{i\in[T]} \in (\mathbb{R}^{d+1})^T$, in the following way: For any $i \in [T-1]$, denoting the center and length of the i^{th} segment $[g_i, g_{i+1}]$ by $c_i = (g_i + g_{i+1})/2$, $l_i = \|g_{i+1} - g_i\|$, and the unit norm vector of direction $\overrightarrow{g_i g_{i+1}}$ by $\overrightarrow{v_i} = (g_{i+1} - g_i)/l_i$, we define the set of triplets $X(\tilde{\mathsf{G}}) = (l_i, c_i, \overrightarrow{v_i})_{i\in[T-1]}$ and its related oriented varifold $\mu_{X(\tilde{\mathsf{G}})} = \sum_{i=1}^{T-1} l_i \delta_{c_i,\overrightarrow{v_i}}$ as in (9). This is a valid discretization of the oriented varifold μ_{G} according to [24, Proposition 1]: $\mu_{X(\tilde{\mathsf{G}})}$ converges towards μ_{G} as the size of the descretization mesh $\sup_{i\in[T-1]} |t_{i+1} - t_i|$ converges to 0.

Finally, we define a distance on discretized time series' graphs $\tilde{\mathsf{G}}_1, \tilde{\mathsf{G}}_2$ as $d_{\mathsf{W}^*}(\tilde{\mathsf{G}}_1, \tilde{\mathsf{G}}_2) = d_{\mathsf{W}^*,3}(X(\tilde{\mathsf{G}}_1), X(\tilde{\mathsf{G}}_2))$.

B.1 Varifold kernels

Denote the one-dimensional Gaussian kernel by $K^{(a)}_\sigma(x, y) = \exp(-|x - y|^2/\sigma)$ for any $(x, y) \in (\mathbb{R}^a)^2$, $a \in \mathbb{N}$ and $\sigma > 0$. In the implementation, we use the following kernels, for any $((t_1, x_1), (t_2, x_2)) \in (\mathbb{R}^{d+1})^2, ((w_1, v_1), (w_2, v_2)) \in (\mathbb{S}^d)^2$,

$$k_{\mathrm{pos}}(x, y) = K^{(1)}_{\sigma_{\mathrm{pos},t}}(t_1, t_2) K^{(d)}_{\sigma_{\mathrm{pos},x}}(x_1, x_2), \quad k_{\mathrm{pos}}(x, y) = K^{(1)}_{\sigma_{\mathrm{dir},t}}(w_1, w_2) K^{(d)}_{\sigma_{\mathrm{dir},x}}(v_1, v_2) \ ,$$

where $\sigma_{\mathrm{pos},t}, \sigma_{\mathrm{pos},x}, \sigma_{\mathrm{dir},t}, \sigma_{\mathrm{dir},x} > 0$ are hyperparameters. In practice, we select $\sigma_{\mathrm{pos},x} \approx \sigma_{\mathrm{dir},x} \approx 1$ when the times series are centered and normalized. Otherwise we select $\sigma_{\mathrm{pos},x} \approx \sigma_{\mathrm{dir},x} \approx \bar{\sigma}_s$ with $\bar{\sigma}_s$ the average standard deviation of the time series. We choose $\sigma_{\mathrm{pos},t} \approx \sigma_{\mathrm{dir},t} = m f_e$ with f_e the sampling frequency of the time series and $m \in [5]$ an integer depending on the time change between the starting and the target time series graph. The more significant the time change, the higher m should be. The intuition comes from the fact that the width $\sigma_{\mathrm{pos},t}, \sigma_{\mathrm{dir},t}$ rules the time windows used to perform the comparison, and $\sigma_{\mathrm{pos},x}, \sigma_{\mathrm{dir},x}$ affects the space window. The size of the windows should be selected depending on the variations in the data.

C Tuning the hyperparameters of the TS-LDDMM kernel given in (7)

The parameter $\sigma_{T,0}$ should be chosen *large* compared the sampling frequency f_e and compared to average standard deviation $\bar{\sigma}_s$ of the time series, e.g $\sigma_{T,0} = 100$ as $\bar{\sigma}_s \approx f_e \approx 1$. It makes the time transformation smoother. If $\sigma_{T,0}$ is too small, for instance, $\sigma_{T,0} = f_e$, the effect of the time deformation is too localized, and there are not enough samples to make it visible.

The parameter $\sigma_{T,1}$ should be of the same order as f_e: two different points in time can have various space transformations. σ_x should be of the same order of $\bar{\sigma}_s$: two points with a big difference regarding space compared to $\bar{\sigma}_s$ can have very different space transformations.

We take $c_0 \approx 10c_1$, we want to encourage time transformation before space transformation. We take $(c_0, c_1) = (1, 0.1)$ in all experiments.

D Numerical details

A report of all the hyperparameters selected is given in Table 3.

D.1 Optimization details of (6)

Initialization At the initialization of (6), all the momentums parameter are set to 0 and the graph of reference is set to the graph of a time series in the dataset having a mediane samples size.

Gradient descent. The chosen gradient descent method is "adabelief" [45] implemented in the library OPTAX[4]. There are two main parameters in the gradient descent: the number of steps nb_steps, and the maximum value of step size η_M. The stepsize has a particular scheduling:

- Warmup period on $0.1\times$ nb_steps steps: the stepsize increases linearly from 0 to η_M. The goal is to learn progressively the parameters. If the stepsize is too large at the start, smaller steps at the end can't make up for the mistakes made at the beginning.
- Fine tuning periode on $0.9\times$ nb_steps : the stepsize decreases from η_M to 0 with a cosine decay implemented in the OPTAX scheduler, i.e. the decreasing factor as the form $0.5(1 + \cos(\pi t/T))$.

The sharper the deformations, the larger the number of steps and the maximum value of step size should be selected. We suggest nb_steps=300, $\eta_M = 0.1$ for small deformations and nb_steps=800, $\eta_M = 0.3$ for big ones (time dilation with a factor $\lambda \geq 2$).

D.2 Synthetic experiments

For any deformations generation in both experiments (well-specified and misspecified), we take $\sigma_{T,0}, \sigma_{T,1}, \sigma_x = (100, 1, 1)$ and $c_0, c_1 = (1, 0.1)$ for the kernel K_{G} and $\sigma_{\mathrm{pos},t}, \sigma_{\mathrm{pos},t}, \sigma_{\mathrm{dir},t}, \sigma_{\mathrm{dir},x} = (2, 1, 2, 0.6)$ for the varifold kernels $k_{\mathrm{pos}}, k_{\mathrm{dir}}$ related to the loss $\mathscr{L}$.

In both experiments, we have nb_steps=300 abd $\eta_M = 0.1$.

D.3 Mouse experiments

The number of steps is larger in the second experiment (before/after injection) because the deformations are sharper.

D.4 Classification experiments

We defined a default parametrization for all classifiers.

For classifiers: CNN, ResNet, Catch22, DTW-KNN, Rocket we used the aeon[5] implementations with their default settings.

For Tloss-SVC we used the implementation provided on github[6] with the following parameters for learning representations: batch_size: 10, channels: 40, depth: 10, nb_steps: 200, in_channels: 1, kernel_size: 3, lr: 0.001, nb_random_samples: 10, negative_penalty: 1, out_channels: 320, reduced_size: 160. We used the Support Vector Classifier (SVC) from scikit-learn with thee regularization term C: 1. Others parameters are set to default.

[4] https://optax.readthedocs.io/en/latest/

[5] https://www.aeon-toolkit.org/en/stable/index.html

[6] https://github.com/mqwfrog/ULTS

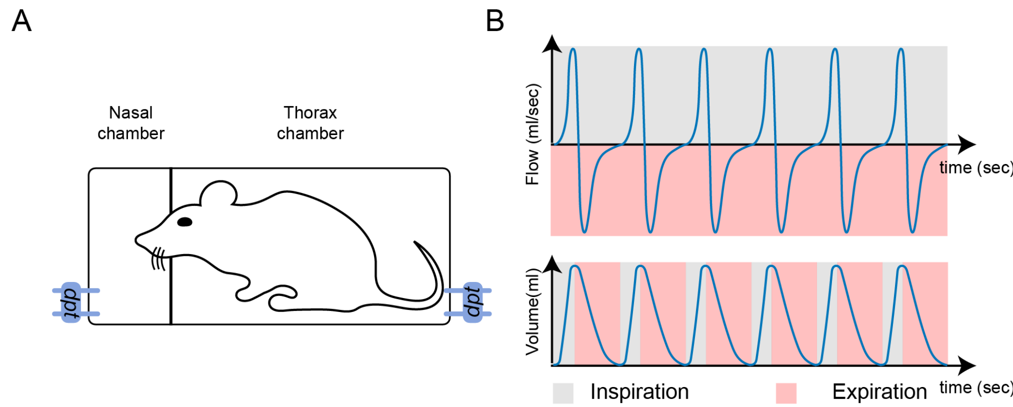

Figure 6: A: Illustration of a double-chamber plethysmograph. The term *dpt* stands for differential pressure transducer which measures the pressure in each compartment, the pressure then being converted to flow. B: Nasal airflow (top) and lung volume (bottom). During inspiration, airflow is positive (grey) and during expiration, airflow is negative (pink).

For TS-LDDMMM-SVC, all kernels' parameters et optimizer parameter are presented in Table 3. As well, we used the Support Vector Classifier from scikit-learn with thee regularization term C: 1. Others parameters are set to default.

Table 3: Parameters used in all the experiments. For synthetic data, K_{G} refers to the kernel used in the generation, which is the same for the estimation only in the well-specified case. $\bar{l}$ refers to the average time series length and N_d refers to the number of dimensions.

objects	Optimizer	$k_{\text{pos}}, k_{\text{dir}}$	K_{G}
Parameter	(nb_steps,η_M)	$(\sigma_{\text{pos},t}, \sigma_{\text{pos},t}, \sigma_{\text{dir},t}, \sigma_{\text{dir},x})$	$(c_0, c_1, \sigma_{T,0}, \sigma_{T,1}, \sigma_x)$
Synthetic data well-specified	(300,0.1)	$(2, 1, 2, 0.6)$	$(1, 0.1, 100, 1, 1)$
Synthetic data misspecified	(300,0.1)	$(2, 1, 2, 0.6)$	$(1, 0.1, 100, 1, 1)$
Mouse before injection	(400,0.3)	$(2, 1, 2, 0.6)$	$(1, 0.1, 100, 1, 1)$
Mouse before/after injection	(800,0.3)	$(5, 1, 5, 0.6)$	$(1, 0.1, 150, 1, 1)$
classification	(400,0.1)	$(\max(2, 0.03\bar{l}), N_d, \max(2, 0.03\bar{l}), 0.6)$	$(1, 0.1, 0.33\bar{l}, 1, N_d)$

E Mouse respiratory dataset

Ventilation is a simple physiological function that ensures a vital supply of oxygen and the elimination of CO2. Acetylcholine (Ach) is a neurotransmitter that plays an important role in muscular activity, notably for breathing. Indeed, muscle contraction information passes from the brain to the muscle through the nervous system. Achs are located in synapses of the nervous system (central and peripheral) and skeletal muscles. They ensure the information transmission from nerve to nerve. However, the transmission cannot end without the hydrolysis of Ach by the enzyme Acetylcholinesterase (AchE), allowing nerves to return to their resting state. Inhibition of (AchE) with, for instance, nerve gas, pesticide, or drug intoxication leads to respiratory arrests.

The dataset comes from the experiment [32], where they studied the consequences of partial deficits in AChE and AChE inhibition on mice respiration. AchE inhibition was induced with an irritant molecule called physostigmine (an AchE inhibitor). Mice nasal airflows were sampled at 2000Hz with a Double Chamber plethysmograph [21], as depicted in Figure 6-A). The flow is expressed in $ml.s^{-1}$; it has a positive value during inspiration and a negative value expiration Figure 6-B). Among the mice population, we selected 7 control mice (**wt**) and 7 ColQ mice (**colq**), which do not have AChE anchoring in muscles and some tissues. As described in [32], mice experiments were as follows:

1. The mouse is placed in a DCP for 15 or 20 min to serve as an internal control.
2. The mouse is removed from the DCP and injected with physostigmine.
3. The mouse is placed back into the DCP, and its nasal flow is recorded for 35 or 40 min.

Respiratory cycles were extracted following procedure [17]. We removed respiratory cycles whose duration exceeds 1 second; the average respiratory cycle duration is 300 ms. We randomly sampled 10 respiratory cycles per minute and mouse. It leads to a dataset of 12,732 (time, genotype)-annotated respiratory cycles.

F Classification datasets

All datasets were taken from UCR/UEA archives [10, 2]. Among all available datasets[7], we selected 4 datasets related to time series shape comparison. All datasets were downloaded with the python package aeon[8] which already includes the train test split. Essential dataset information is summarized in Table 4.

Table 4: Time series datasets summary for shape based classification.

Dataset	Train size	test size	Lenghth	Number of classes	Number of dimensions	Type
ArrowHead	36	175	251	3	1	IMAGE
ECG200	100	100	96	2	1	ECG
GunPoint	50	150	150	2	1	MOTION
NATOPS	180	180	51	6	24	MOTION

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[7]https://timeseriesclassification.com

[8]https://www.aeon-toolkit.org/en/stable/

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