Shapes analysis for time series.

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Abstract

Analyzing inter-individual variability of physiological functions is particularly appealing in medical and biological contexts to describe or quantify health conditions. Such analysis can be done by comparing individuals to a reference one with time series as biomedical data. This paper introduces an unsupervised representation learning (URL) algorithm for time series tailored to inter-individual studies. The idea is to represent time series as deformations of a reference time series. The deformations are diffeomorphisms parameterized and learned by our method called TS-LDDMM. Once the deformations and the reference time series are learned, the vector representations of individual time series are given by the parametrization of their corresponding deformation. At the crossroads between URL for time series and shape analysis, the proposed algorithm handles irregularly sampled multivariate time series of variable lengths and provides shape-based representations of temporal data. In this work, we establish a representation theorem for the graph of a time series and derive its consequences on the LDDMM framework. We showcase the advantages of our representation compared to existing methods using synthetic data and real-world examples motivated by biomedical applications.

1 Introduction

Our goal is to analyze the inter-individual variability within a time series dataset, an approach of significant interest in physiological contexts [23, 55, 4, 19]. Specifically, we aim to develop an unsupervised feature representation method that encodes the specificities of individual time series in comparison to a reference time series. In physiology, examining the various "shapes" in a time series related to biological phenomena and their variations due to individual differences or pathological conditions is common. However, the term "shape" lacks a precise definition and is more intuitively understood as the silhouette of a pattern in a time series. In this paper, we refer to the shape of a time series as the graph of this signal.

Although community structures with representatives can be learned in an unsupervised manner [52, 37] using contrastive loss [18, 51, 37] or similarity measures [2, 19, 43, 58], the study of inter-individual variability of shapes within a cluster [40, 48] remains an open problem in unsupervised representation learning (URL), particularly for *irregularly sampled* time series with *variable lengths*.

Our work explicitly focuses on learning shape-based representation of time series. First, we propose to view the shape of a time series not merely as its curve $\{s_t : \ t \in \mathsf{I}\}$, but as its graph $\mathsf{G}(s) = \{(t, s(t)) : \ t \in \mathsf{I}\}$. Then, building on the shape analysis literature [5, 54], we adopt the Large Deformation Diffeomorphic Metric Mapping (LDDMM) framework [5, 54] to analyze these graphs. The core idea is to represent each element $\mathsf{G}(s^j)$ of a dataset $(s^j)_{j\in[N]}$ as the transformation of a reference graph $\mathsf{G}(\mathbf{s}_0)$ by a diffeomorphism ϕ_j, i.e. $\mathsf{G}(s^j) \sim \phi_j.\mathsf{G}(\mathbf{s}_0)$. The diffeomorphism ϕ_j 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

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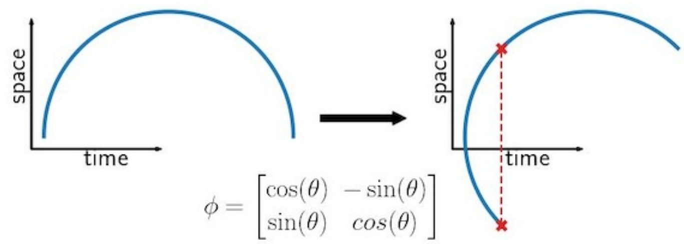


Figure 1: A time series' graph $\mathsf{G} = \{(t, s(t)) : \ t \in \mathsf{I}\}$ can lose its structure after applying a general diffeomorphism $\phi.\mathsf{G}$: a time value can be related to two values on the space axis.

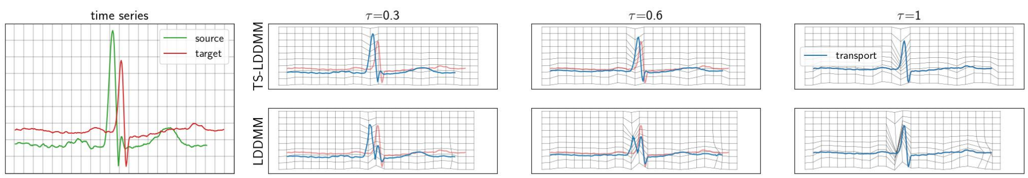


Figure 2: LDDMM and TS-LDDMM are applied to ECG data. We observe that LDDMM, using a general Gaussian kernel, does not learn the time translation of the first spike but changes the space values, i.e., one spike disappears before emerging at a translated position. At the same time, TS-LDDMM handles the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

representation features of the graphs $(\mathsf{G}(s^j))_{j\in[N]}$. Finally, these shape-encoding features can be used as inputs to any statistical or machine-learning model.

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 curve [21]. Our contributions arise from this observation: we specify the class of diffeomorphisms to consider and show how to learn them. This change is fruitful in representing transformations of time series graphs as illustrated in Figure 2.

Our contributions can be summarized as follows:

- We propose an unsupervised method (TS-LDDMM) to analyze the inter-individual variability of shapes in a time series dataset (Section 4). In particular, the method can handle multivariate time series *irregularly sampled* and with *variable sizes*.
- We 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 concerning its hyperparameters (**??**), also providing guidelines for tuning (Appendix D).
- We highlight the *interpretability* of TS-LDDMM for studying the inter-individual variability in a clinical dataset (Section 5).
- We illustrate the quantitative interest of such representation on classification tasks on real shape-based datasets with regular and irregular sampling (**??**).

2 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.

3 Background on LDDMM

In this part, we expose how to learn the diffeomorphisms $(\phi_j)_{j\in[N]}$ using LDDMM, initially introduced in [5]. 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, time series are going to be represented by diffeomorphism parameters $(\alpha_j)_{j\in[N]}$. That is why LDDMM is chosen since it offers a parametrization for diffeomorphisms that 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 continuous 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 [20, 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 [38] to interpret V as a tangent space relative to the group of diffeomorphisms $\mathsf{H} = \{\phi^v :\ v \in \mathrm{L}^2([0,1],\mathsf{V})\}$. Following this geometric point of view, geodesics can be constructed on H by using the following squared norm

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

By deriving differential constraints related to the minimum of (2) and using Cauchy-Lipschitz conditions, geodesics can be defined only by giving the starting point and the initial velocity $v_0 \in \mathsf{V}$ [38], as straight lines in Euclidean space. Denoting by $w(v_0)$ the geodesic starting from the identity with inital velocity v_0, the exponential map is defined as $\varphi^{\{v_0\}} \triangleq \phi^v$ and the previous matching problem becomes a *geodesic shooting problem*:

$$\inf_{v_0\in\mathsf{V}} \mathscr{L}(\varphi^{\{v_0\}}.\mathbf{x},\mathbf{y}). \tag{3}$$

Using $\varphi^{\{v_0\}}$ instead of ϕ^v for any $v \in \mathrm{L}^2([0,1],\mathsf{V})$ regularizes the problem and induces a sparse representation for the learning diffeomorphisms. Moreover, by setting V as an RKHS, the geodesic shooting problem has a unique solution and becomes tractable, as described in the next section.

Discrete parametrization of diffeomorpshim. In this part, V is chosen as an RKHS [6] generated by a smooth kernel K (e.g., Gaussian). We follow [15] and define a discrete parameterization of the velocity fields to perform geodesics shooting (3). 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 $x \in \mathbb{R}^{d'}$,

$$v_0\left(\alpha_0, \mathsf{X}_0\right)(x) = \sum_{k=1}^{\mathbf{n}_0} K(x, x_{k,0})\alpha_{k,0}\ . \tag{4}$$

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

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?)** [38] show that the velocity field v of the solution of (3) keeps the same structure along time, such that for any $x \in \mathbb{R}^{d'}$ and $\tau \in [0,1]$,

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

$$\begin{cases} \frac{\mathrm{d}x_k(\tau)}{\mathrm{d}\tau} = v_\tau(x_k(\tau)) \ , \quad \frac{\mathrm{d}\alpha_k(\tau)}{\mathrm{d}\tau} = -\sum_{k=1}^{\mathbf{n}_0} \mathrm{d}_{x_k(\tau)} K(x_k(\tau), x_l(\tau))\alpha_l(\tau)^\top \alpha_k(\tau) \\ \alpha_k(0) = \alpha_{k,0}, \quad x_k(0) = x_{k,0} \ , k \in [\mathbf{n}_0] \end{cases} \tag{5}$$

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 (5), 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:

$$\mathcal{F}_{\mathbf{x},\mathbf{y}} : (\alpha_k)_{k\in[T_1]} \mapsto \mathscr{L}\left(\varphi^{\{v_0\}}.\mathbf{x}, \mathbf{y}\right) + \lambda||v_0||_{\mathsf{V}}^2 \ , \tag{6}$$

where v_0 is defined by (4) and $\varphi^{\{v_0\}}.\mathbf{x}$ is the result of the numerical integration of (5) 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 [45, 30] (NF) or their continuous counterpart [11, 22, 46] (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 [17, 14]. 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.

4 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 $\tilde{s}^j = (\tilde{s}_i^j = s^j(t_i^j))_{i\in[n_j]}$ collected at timestamps $(t_i^j)_{i\in[n_j]}$ for any $j \in [N]$. Note that **the number of samples n_j is not necessarily the same across 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 [57, 35].

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 [54], 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 $j \in [N]$,

$$\phi_j.\mathsf{G}(\mathbf{s}_0) = \{\phi_j\,(t, \mathbf{s}_0(t))\,,\ t \in \mathsf{I}\} \ . \tag{7}$$

$\mathbf{s}_0$ 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 (7). 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 (7) boils down solving:

$$\mathrm{argmin}_{\tilde{\mathsf{G}}_0, (\alpha_k^j)_{k\in[\mathbf{n}_0]}^{j\in[N]}} \sum_{j=1}^{N} \mathcal{F}_{\tilde{\mathsf{G}}_0, \mathbf{y}_j} \left((\alpha_k^j)_{k\in[\mathbf{n}_0]} \right) \ , \tag{8}$$

which is carried out by 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 E.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, (8) asks to define a kernel and a loss in order to perform geodesic shooting (6), which is the purpose of the following subsection.

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

This section presents 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 graphs have more structure than a simple 1D curve [21] and deserve their unique analysis, which will prove fruitful as demonstrated in Section 5.

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 with 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 B.

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. *Note 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 (6) on $\mathbb{R}^{d+1}$, we consider for V the RKHS associated with the kernel defined for any $(t,x),(t',x') \in (\mathbb{R}^{d+1})^2$:

$$K_{\mathsf{G}}((t,x),(t',x')) = \begin{pmatrix} c_0 K_{\text{time}} & 0 \\ 0 & c_1 K_{\text{space}} \end{pmatrix} \,, \tag{9}$$
$$K_{\text{space}} = K_{\sigma_{T,1}}^{(1)}(t,t') K_{\sigma_x}^{(d)}(x,x') \mathrm{I}_d \,, K_{\text{time}} = K_{\sigma_{T,0}}^{(1)}(t,t') \,,$$

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* (5) *with v_0 satisfying* (4)*, there exist $\gamma \in \mathsf{D}(\mathbb{R})$ and $f \in \mathrm{C}^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$ such that $\phi^v = \Psi_\gamma \circ \Phi_f$.*

Instead of Gaussian kernels, other types of smooth kernels can be selected as long as the structure (9) is respected.

Remark 3. *With this choice of kernel, the features associated with 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* (4) *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 D, 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 (6).

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) [16, 7], 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 [28]. 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 C.

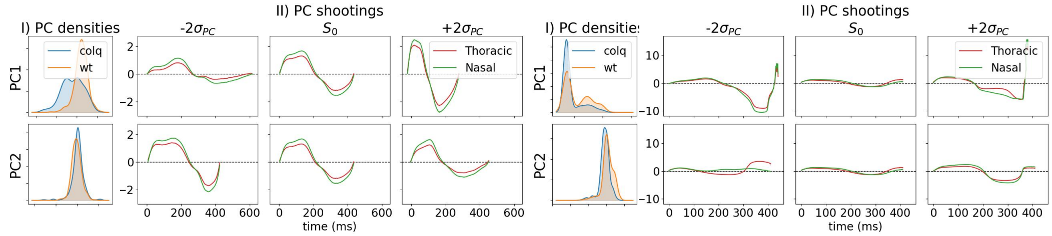
More precisely, given two sets $\mathsf{G}_0 = (g_i^0)_{i\in[T_0]}, \mathsf{G}_1 = (g_i^1)_{i\in[T_1]} \in (\mathbb{R}^{d+1})^{T_1}$ and a kernel[2] $k : (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2 \to \mathbb{R}$ verifying [28, Proposition 2 & 4], for any $\xi \in \{0,1\}$ and $i \in [T_\xi - 1]$, denoting 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 $\overrightarrow{v_i}^\xi = (g_{i+1}^\xi - g_i^\xi)/l_i^\xi$, the varifold distance between G_0 and G_1 is defined as,

$$d_{\mathsf{W}^*}^2(\mathsf{G}_0, \mathsf{G}_1) = \sum_{i,j=1}^{T_0-1} l_i^0 k((c_i^0, \overrightarrow{v_i}^0), (c_j^0, \overrightarrow{v_j}^0)) l_j^0 - 2 \sum_{i=1}^{T_0-1} \sum_{j=1}^{T_1-1} l_i^0 k((c_i^0, \overrightarrow{v_i}^0), (c_j^1, \overrightarrow{v_j}^1)) l_j^1$$
$$+ \sum_{i,j=1}^{T_1-1} l_i^1 k((c_i^1, \overrightarrow{v_i}^1), (c_j^1, \overrightarrow{v_j}^1)) l_j^1$$

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

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

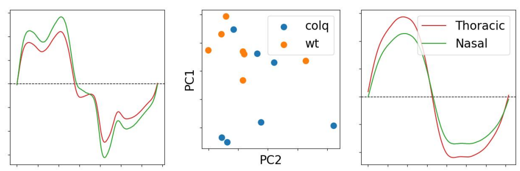
[2] $\mathbb{S}^d = \{x \in \mathbb{R}^{d+1} : \ |x| = 1\}$



(a) TS-LDDMM

(b) LDDMM

Figure 3: Analysis of the two principal components (PC) related to mice' respiratory cycles before exposure for TS-LDDMM Figure 3a, and LDDMM Figure 3b. In both cases, I) displays PC densities according to mice genotype and II) displays deformations of the reference graph S_0 along each PC.



(a) colq cycle (b) PC1 vs PC2 (c) wt cycle

Figure 4: Figure 4a is a **colq** respiratory cycle. Figure 4b displays individual mouse reference respiratory cycle in the TS-LDDMM PC1-PC2 coordinates. Figure 4c is a referent respiratory cycle of a **wt** mouse learned with TS-LDDMM.

Note that the loss kernel k has nothing to do with the velocity field kernel denoted by K_{G} or K specified in Section 4.1. Finally, we define the data fidelity loss function, $\mathscr{L}$, as a sum of $d^2_{\mathsf{W}^*}$ using different kernel's width parameters σ to incorporate multiscale information. $\mathscr{L}$ is indeed differentiable with respect to its first variable. The specific kernels $k_{\mathrm{pos}}, k_{\mathrm{dir}}$ that we use in our experiments are given Appendix C.1. For further readings on curves and surface representation as varifolds, readers can refer to [28, 10].

5 Experiments

For conciseness, several experiments are relegated in appendix:

1. **TS-LDDMM representation identifiability, ??:** On synthetic data, we evaluate the ability of our method to retrieve the parameter v_0^* that encodes the deformation $\varphi^{\{v_0^*\}}$ acting on a time series graph G by solving the geodesic shooting problem (6) between G and $\varphi^{\{v_0^*\}}.\mathsf{G}$. **Results** show that TS-LDDMM representations are identifiable or weakly identifiable depending on the velocity field kernel K_G specification.

2. **Robustness to irregular sampling** We compare the robustness of TS-LDDMM representation with 9 URL methods handling irregularly sampled multivariate time series on 15 shape-based datasets (7 univariates & 8 multivariates). We assess methods' classification performances under regular sampling (0% missing rate) and three irregular sampling regimes (30%, 50%, and 70% missing rates), according to the protocol depicted in [29]. **Results** show that our method, TS-LDDMM, outperforms all methods for sampling regimes with missing rates: 0%, 30%, and 50%.

3. **Classification benchmark on regularly sampled datasets, ??:** We compare performances of a kernel support vector machine (SVC) algorithm based on TS-LDDMM representation with 3 state-of-the-art classification methods from shape analysis on 15 shape-based datasets (7 univariates & 8 multivariates). **Results** show that the TS-LDDMM-based method outperforms other methods (best performances over 13 datasets), making TS-LDDMM representation relevant for time series shape analysis.

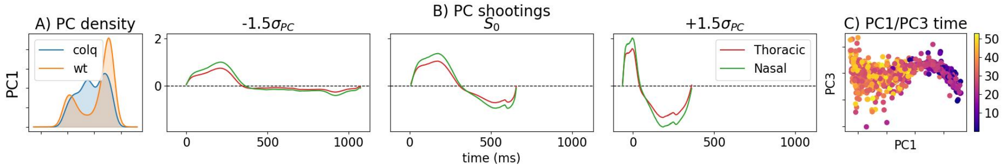


Figure 5: Analysis of the first Principal Component (PC1) related to mice' respiratory cycles before and after exposure for TS-LDDMM. Figure A) displays PC densities according to mice genotype, Figure B) displays deformations of the reference graph S_0 along PC1, and Figure C) displays respiratory cycles with respect to time in PC1 and PC3 coordinates

5.1 Interpretability: analysis of respiratory behavior in mice

This experiment highlights the *interpretability* of TS-LDDMM representation for studying the inter-individual variability in time series biomedical datasets. We consider a multivariate time series dataset that accounts for mice's nasal and thoracic airflow evolution when exposed to an irritant molecule altering respiratory functions [39]. 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, airflows were 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 F.1.

Protocol. For both experiments and representations (TS-LDDMM and LDDMM), we derive the reference respiratory cycle's graph S_0 and the representations $(\alpha_j)_{j\in[N]}$ related to N respiratory cycles extracted according to the procedure [19] by solving (8). Then, we perform a kernel PCA on the initial velocity field $(v_0(\alpha_j, S_0))_{j\in[N]} \in \mathsf{V}^{N_1}$ defined in (4) to breathing behavior. The first experiment includes $N_1 = 700$ respiratory cycles collected before exposure. The second experiment includes $N_2 = 1400$ respiratory cycles with 25% (resp. 75%) before (resp. after) exposure. Appendix G.1 describes methods settings. Essentially, varifold losses are identical for both methods, and the velocity field kernels are set to encompass time and space scales.

Breathing behaviors before exposure. We focus on the analysis of the two first Principal Components (PC) for TS-LDDMM (Figure 3a), and LDDMM (Figure 3b). A respiratory cycle is an inspiration (positive flow) followed by an expiration (negative flow); Figure 4c displays an example of **wt** mouse respiratory cycle. Figure 3 shows that principal components learned with TS-LDMM lead to deformations that remain respiratory cycles, while deformations learned with LDDMM are challenging to interpret as respiratory cycles. The LDDMM velocity field kernel is a Gaussian anisotropic kernel that accounts for time and space scales; however, the entanglement of time and space dimensions in the kernel does not guarantee the graph structure, and it makes the convergence of the method difficult (relative varifold loss error: TS-LDDMM: 0.06, LDDMM: 0.11). Regarding TS-LDDMM, Figure 3a shows its principal components refer to different types of deformations. By interpreting Figure 3a: PC1 accounts for time warping, PC2 expresses the trade-off between inspiration and expiration duration. Compared to **wt** mice, the distribution of **colq** mice feature along the PC1 axis has a heavy left tail, and the associated deformation (-2 σ_{PC}) shows an inspiration with two peaks. Figure 4a shows an example of such respiratory cycles, which may be caused by motor impairment due to enzyme deficiency [19]. Finally, Figure 4b shows that PC1 and PC2 capture the main differences between the two groups as their respective reference graphs S^j are located in different parts of the space.

Breathing behaviors' evolution after exposure to the irritant molecule TS-LDDMM representation features are learned on a dataset that includes respiratory cycles before and after exposure. Figure 5 displays 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 (-1.5 σ_{PC}) leads to longer respiratory cycles that include a pause between inspiration and expiration as observed in [19]. Conjointly, Figure 5-A) shows a bimodal distribution for **wt** mice whereas **wt**' distributions before exposure were unimodal (Figure 3a). Indeed, the irritant molecule inhibits the action of the deficient enzyme, **wt** mice strongly react to the irritant molecule, whereas **colq** mice better adapt due to their deficiency [19].

Result summary. By comparing the shape of individual respiratory cycles, we show that TS-LDDMM features can encode genotype distinctive breathing behaviors and their evolution after exposure to the irritant molecule contrary to LDDMM [21].

6 Related Works

Shape analysis focuses on statistical analysis of mathematical objects invariant under some deformations like rotations, dilations, or time parameterization. The main idea is to represent these objects in a complete Riemannian manifold $(\mathcal{M}, \mathbf{g})$ with a metric $\mathbf{g}$ adapted to the geometry of the problem [38]. Then, any set of points in $\mathcal{M}$ can be represented as points in the tangent space of their Frechet mean $\mathbf{m}_0$ [42, 31] by considering their logarithms. The goal is to find a well-suited Riemannian structure according to the nature of the studied object.

LDDMM framework is a relevant shape analysis tool to represent curves as depicted in [21]. However, graphs of time series are a well-structured type of curve due to the inclusion of the temporal dimension that requires specific care (Figure 1). In a similar vein, Qiu *et al* [44] proposes a method for tracking anatomical shape changes in serial images using LDDMM. They include temporal evolution, but not for the same purpose: the aim is to perform longitudinal modeling of brain images.

Leaving the LDDMM representation, the results of [50, 24] address the representation of curves with the Square-Root Velocity (SRV) representation. However, the SRV representation is applied after reparametrization of the temporal dimension of the unit length segment. Consequently, the graph structure of the time series is not respected, and the original time evolution of the time series is not encoded in the final representation. Very recently, in a functional data analysis framework, a paper [56] (Shape-FPCA) improved by representing the original time evolution. Nevertheless, this method is made for *continuous objects* and only applies to time series of *same length*, making the estimation more sensitive to noise.

Balancing between discrete and continuous elements is a challenging task. In the deep learning literature [11, 29, 53, 27, 34, 1], Neural Ordinary Differential Equations (Neural ODEs) [11] learn continuous latent representations using a vector field parameterized by a neural network, serving as a continuous analog to Residual Networks [59]. This approach was further enhanced by Neural Controlled Differential Equations (Neural CDEs) [29] for handling irregular time series, functioning as continuous-time analogs of RNNs [47]. Extending Neural ODEs, Neural Stochastic Differential Equations (Neural SDEs) introduce regularization effects [34], although optimization remains challenging. Leveraging techniques from continuous-discrete filtering theory, Ansari et al. [1] applied successfully Neural SDEs to irregular time series. Oh *et al.* [41] improved these results by incorporating the concept of controlled paths into the drift term, similar to how Neural CDEs outperform Neural ODEs. With TS-LDDMM, the representation is also derived from an ODE, but the velocity field is parameterized with kernels and optimized to have a minimal norm, which enhances interpretability.

All these state-of-the-art methods previously mentionned [21, 41, 56, 24] are compared to TS-LDDMM in **??**.

7 Limitations and conclusion

Limitations While TS-LDDMM performs well on shape-based datasets, it assumes a certain degree of homogeneity with the existence of a reference time series graphG_0. Extending TS-LDDMM to more heterogeneous datasets using clustering is ongoing work. TS-LDDMM employs kernel computations, which require specific libraries (e.g., KeOps [9]) to be efficient and scalable. However, in our experiments, the time complexity of TS-LDDMM is comparable to that of competitors. It is clear that TS-LDDMM needs to be extended to handle very large datasets with high-dimensional time series (such as videos). Additionally, TS-LDDMM requires tuning several hyperparameters, though this is a common requirement among competitors [21, 41, 56, 24]. In future work, adaptive methods are expected to be developed to provide a more user-friendly interface.

Conclusion This paper proposes a feature representation method, TS-LDDMM, designed for shape comparison on 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 relegated for future work.

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A Societal impact

We believe that the paper has a positive societal impact for the following reasons:

- TS-LDDMM is an interpretable method for understanding inter-individual variability in biomedical datasets, potentially offering new insights in medicine.
- TS-LDDMM bridges the gap between the shape analysis community and the unsupervised representation learning (URL) community, fostering potential future collaborations between these fields.

However, the computational cost of the method may raise environmental concerns similar to those associated with deep learning [41]. Additionally, while TS-LDDMM has promising biomedical applications, it could also be misused for creating poison.

B 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 :

$$\Pi_{\gamma,f}.\mathsf{G}(\mathbf{s}_0) = \{(\gamma(t), f(t, \mathbf{s}_0(t))),\ t \in \mathsf{I}\}$$

$$= \left\{ \left(t, f\left(\gamma^{-1}(t), \mathbf{s}_0(\gamma^{-1}(t))\right)\right),\ t \in \gamma(\mathsf{I}) \right\} . \tag{10}$$

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 (10), 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* (5) *with* v_0 *satisfying* (4)*, 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 (5) with v_0 satisfying (4). 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 [20, 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 $\phi^v = \Psi_\gamma \circ \Phi_f$. □

C 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 [28, 10]. 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 $\omega : \mathbb{R}^{d+1} \times \mathbb{S}^d \to \mathbb{R}$,

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

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 [28, 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 $k_{\text{dir}} > 0$ and k_{pos} which admits an RKHS W_{pos} dense in the space of continous function on $\mathbb{R}^{d+1}$ vanishing at infinite [8].

Given such a kernel $k : (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2 \to \mathbb{R}$ verifying [28, 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

$$\mu_X = \sum_{i=1}^{T_0} l_i \delta_{(x_i, \overrightarrow{v}_i)}, \mu_Y = \sum_{i=1}^{T_1} l'_i \delta_{(y_i, \overrightarrow{w}_i)} , \tag{11}$$

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 (11). This is a valid discretization of the oriented varifold μ_{G} according to [28, 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 $d_{\mathsf{W}^*}(\tilde{\mathsf{G}}_1, \tilde{\mathsf{G}}_2) = d_{\mathsf{W}^*,3}(X(\tilde{\mathsf{G}}_1), X(\tilde{\mathsf{G}}_2))$.

C.1 Varifold kernels

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 $\sigma > 0$. 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.

D Tuning the hyperparameters of the TS-LDDMM velocity field kernel

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

E Experimental settings

All experiments were performed on a Debian 6.1.69-1 server with NVIDIA RTX A2000 12GB GPU, Intel(R) Xeon(R) Gold 5220R CPU @ 2.20GHz, and 250 GB of RAM. The source code will be available on Github.

E.1 Optimization details of TS-LDDMM & LDDMM

We implemented TS-LDDMM in Python with the JAX library [3].

Initialization. As initialization of (8), all momentum parameters are set to 0, and the initial graph of reference is picked from the dataset such that its length is equal to the median length observed in the dataset.

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

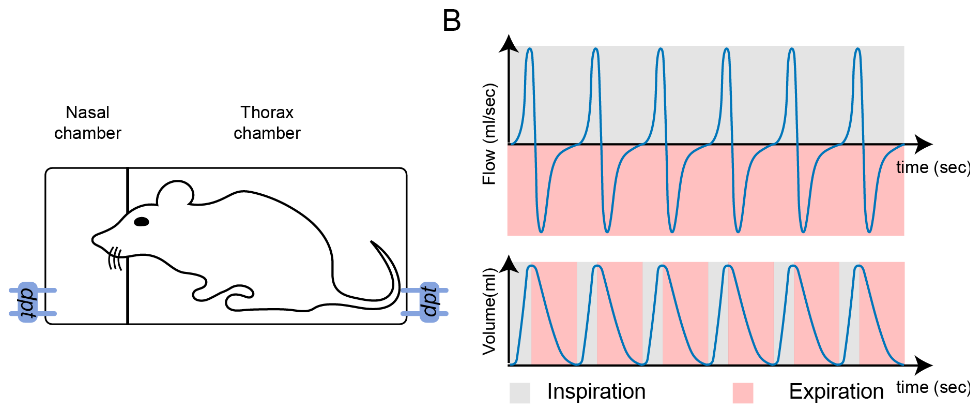

Figure 6: A: Illustration of a double-chamber plethysmograph. The term *dpt* stands for differential pressure transducer which measures the pressure in each compartment, the pressure then being converted to flow. B: Nasal airflow (top) and lung volume (bottom). During inspiration, airflow is positive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

Gradient descent. The chosen gradient descent method is "adabelief" [60] implemented in the OPTAX library [4]. The gradient descent has two main parameters: the number of steps (nb_steps) and the maximum stepsize value (η_M). The stepsize has a scheduling scheme:

- 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 step size is too large at the start, smaller steps at the end cannot 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 $0.5(1 + \cos(\pi t/T))$.

By default, we set nb_steps to 400 and η_M to 0.1.

F Datasets

F.1 Mouse respiratory cycle 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 [39], 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 [26], 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 [39], mice experiments were as follows:

1. The mouse is placed in a DCP for 15 or 20 min to serve as an internal control.

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

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 [19]. 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.2 Shape-based UCR/UEA time series classification datasets

We selected 15 shape-based datasets (7 univariates and 8 multivariates) from the from the University of East Anglia (UEA) and the University of California Riverside (UCR) Time Series Classification Repository[5] [13, 3]. All datasets were downloaded with the python package aeon[6]. Essential datasets information are summarized in Table 1 and further can be found in [13, 3].

Table 1: UCR/UEA shape-based time series datasets for classification.

	Dataset	Size	Lengh	Number of classes	Number of dimensions	Type
Univariate	ArrowHead	211	251	3	1	IMAGE
	BME	180	128	3	1	SIMULATED
	ECG200	200	96	2	1	ECG
	FacesUCR	2250	131	14	1	IMAGE
	GunPoint	200	150	2	1	MOTION
	PhalangesOutlinesCorrect	2658	80	2	1	IMAGE
	Trace	200	275	4	1	SENSOR
Multivariate	ArticularyWordRecognition	575	144	25	9	SENSOR
	Cricket	180	1197	12	6	MOTION
	ERing	60	65	6	4	SENSOR
	Handwriting	1000	152	26	3	MOTION
	Libras	360	45	15	2	VIDEO
	NATOPS	360	51	6	24	MOTION
	RacketSports	303	30	4	6	SENSOR
	UWaveGestureLibrary	240	315	8	3	SENSOR

G Appendix for experiment: Analysis of respiratory behavior in mice

G.1 Settings

This experiment involves TS-LDDMM and LDDMM [21] methods. Both methods are run twice, first on respiratory cycles before exposure to the irritant molecule to capture mice breathing behavior at rest and on all respiratory cycles to capture the influence of the irritant molecule. Exposure to the irritant molecule leads to significant shape deformation in the respiratory cycles, and the terms must be added to the varifold loss to capture deformations at a large time scale.

TS-LDDMMM parameters.

- **Before exposure:** The velocity field kernel K_G is set to $(c_0, c_1, \sigma_{T,0}, \sigma_{T,1}, \sigma_x) = (1, 0.1, 150, 1, 2)$. The varifold loss is the sum of three varifolds to capture shapes variations at different scales with parameters: (Varifold 1,Varifold 2,Varifold 3): $((5, 2, 5, 1), (2, 1, 2, 0.6), (1, 0.6, 1, 0.6))$ and the mapper $(\sigma_{\mathrm{pos},t}, \sigma_{\mathrm{pos},t}, \sigma_{\mathrm{dir},t}, \sigma_{\mathrm{dir},x})$. The optimizer has 800 steps with a maximum stepsize η_M of 0.3.
- **Before/after exposure:** The velocity field kernel K_G is set to $(c_0, c_1, \sigma_{T,0}, \sigma_{T,1}, \sigma_x) = (1, 0.1, 220, 1, 2)$. The varifold loss is the sum of four varifolds to capture shapes variations at different scales with parameters: (Varifold 1,Varifold 2,Varifold 3, Varifold 4): $((30, 2, 30, 1), (5, 2, 5, 1), (2, 1, 2, 0.6), (1, 0.1, 1, 0.1))$ and the mapper $(\sigma_{\mathrm{pos},t}, \sigma_{\mathrm{pos},t}, \sigma_{\mathrm{dir},t}, \sigma_{\mathrm{dir},x})$. The optimizer has 800 steps with a maximum stepsize η_M of 0.3.

[5]https://timeseriesclassification.com
[6]https://www.aeon-toolkit.org/en/stable/

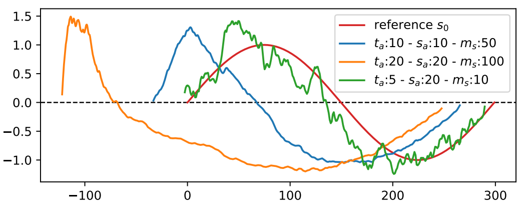

Figure 7: Plots of $\varphi^{\{v_0(\alpha^*, \mathsf{X})\}}.\mathsf{X}$ for different values of α^* according to its sampling parameter t_a, s_a, m_s, taking $\mathsf{X} = \mathsf{G}(s_0)$ with $s_0 : k \in [300] \to \sin(2\pi k/300)$.

Table 2: 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

LDDMMM parameters. Note that varifold losses are unchanged between TS-LDDMM and LDDMM. Compared to TS-LDDMM, the convergence of LDDMM is more sensitive to the maximum stepsize η_m, which must remain small for LDDMM to guarantee the convergence.

- **Before exposure:** The velocity field kernel K_G is an anysotropic Gaussian kernel with parameters $\sigma_T = 150$ for the time dimension and $\sigma_x = 2$ for space dimensions. The varifold loss is the sum of three varifolds to capture shapes variations at different scales with parameters: (Varifold 1,Varifold 2,Varifold 3): $((5, 2, 5, 1), (2, 1, 2, 0.6), (1, 0.6, 1, 0.6))$ and the mapper $(\sigma_{\text{pos},t}, \sigma_{\text{pos},t}, \sigma_{\text{dir},t}, \sigma_{\text{dir},x})$. The optimizer has 800 steps with a maximum stepsize η_M of 0.01.
- **Before/after exposure:** The velocity field kernel K_G is an anysotropic Gaussian kernel with parameters $\sigma_T = 220$ for the time dimension and $\sigma_x = 2$ for space dimensions. The varifold loss is the sum of four varifolds to capture shapes variations at different scales with parameters: (Varifold 1,Varifold 2,Varifold 3, Varifold 4): $((30, 2, 30, 1), (5, 2, 5, 1), (2, 1, 2, 0.6), (1, 0.1, 1, 0.1))$ and the mapper $(\sigma_{\text{pos},t}, \sigma_{\text{pos},t}, \sigma_{\text{dir},t}, \sigma_{\text{dir},x})$. The optimizer has 800 steps with a maximum stepsize η_M of 0.01.

H Appendix for experiment: TS-LDDMM representation identifiability

H.1 Settings

This experiment only involves the TS-LDDMM method in two different settings:

- **The velocity field kernel K_G is well-specified:** The velocity field kernel K_G is set to $(c_0, c_1, \sigma_{T,0}, \sigma_{T,1}, \sigma_x) = (1, 0.1, 100, 1, 1)$, the varifold loss kernels (k_{pos}, k_{dir}) are set to $(\sigma_{\text{pos},t}, \sigma_{\text{pos},t}, \sigma_{\text{dir},t}, \sigma_{\text{dir},x}) = (2, 1, 2, 0.6)$, and the optimizer has 400 steps with a maximum stepsize η_M of 0.05.
- **The velocity field kernel K_G is missspecified:** The velocity field kernel K_G is set with $(c_0, c_1, \sigma_{T,1}) = (1, 0.1, 1)$, $\sigma_{T,0}$ ranging in $(1, 5, 10, 50, 100, 200, 300)$, and σ_x ranging in $(0.1, 1, 10, 100)$. The varifold loss kernels (k_{pos}, k_{dir}) are set to $(\sigma_{\text{pos},t}, \sigma_{\text{pos},t}, \sigma_{\text{dir},t}, \sigma_{\text{dir},x}) = (2, 1, 2, 0.6)$, and the optimizer has 400 steps with a maximum stepsize η_M of 0.05.

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 (6).

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 **??**. We fix the initial control points 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 (4) with initial momentums α^* and control points X, we apply the induced deformation $\varphi^{\{v_0\}}$ by (5) to X and obtain $\varphi^{\{v_0\}}.\mathsf{X}$. Finally, we solve (6) 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 (6) 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 7: 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 (6). We observe in Table 2 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 C.1-D, we propose guidelines to drive future hyperparameters tuning and further discussions related to $\sigma_{T,1}, c_0, c_1$.

I Appendix for experiment: Robustness to irregular sampling

This experiment is inspired by [41] where the authors perform an extensive comparison of Neural Ordinary Differential Equations (Neural ODEs) methods [29]. We assess the classification performances of several methods under regular sampling (0% missing rate) and three irregular sampling regimes on 15 shape-based datasets (7 univariate & 8 multivariate). Methods and training strategy are taken from its associated Github[7] and described in what follows. We conclude with the results, which show that our method, TS-LDDMM, outperforms all methods for sampling regimes with missing rates: 0%, 30%, and 50%.

I.1 Benchmark methods

In related work, we give an overview of Neurals ODEs methods and their relation with TS-LDDMM.

- RNN-based methods: Baseline reccurent neural networks including RNN [36], LSTM [25], and GRU [12].
- Attention-based methods: Multi-Time Attention Networks (MTAN) [49] and Multi-Integration Attention Module (MIAM) [33]. Both handle multivariate time series irregularly sampled with attention mechanisms.
- Neural ODEs: ODE-LSTM [32] a form of Neural-ODEs used to learn continuous latent representations.

[7] `https://github.com/yongkyung-oh/Stable-Neural-SDEs`

- Neural SDEs: Neural SDE [34] and Neural LNSDE [41] have been proposed to model randomness in time-series using drift and diffusion terms as an extension of Neural-ODEs.
- Shape-Analysis methods: TS-LDDMM (ours) and LDDMM [21]. From shape analysis, both methods learn representations by solving ODEs parametrized with Kernels. While both methods handle multivariate signals irregularly sampled, TS-LDDMM is specifically designed for time series.

I.2 Model architecture

Neural ODEs methods As depicted in [41], any Neural ODEs layer in Appendix I.1 is followed by an MLP with two fully connected layers with `ReLU` activations. The risk of overfitting and the model regularization are handled with a dropout rate of 10% and an early-stopping mechanism, ceasing the training when the validation loss does not improve for 10 successive epochs.

TS-LDDMM and LDDMM

I.3 Protocol

I.4 Results

Methods	Test F1-score			
	Regular	**30 % dropped**	**50 % dropped**	**70 % dropped**
RNN (1999)	0.64 ± 0.21	0.53 ± 0.23	0.48 ± 0.21	0.44 ± 0.21
LSTM (1997)	0.61 ± 0.29	0.57 ± 0.29	0.53 ± 0.25	0.51 ± 0.29
GRU (2014)	0.71 ± 0.26	0.68 ± 0.28	0.66 ± 0.28	$\underline{0.59 \pm 0.28}$
MTAN (2021)	0.59 ± 0.28	0.58 ± 0.28	0.54 ± 0.29	$\underline{0.51 \pm 0.28}$
MIAM (2022)	0.48 ± 0.35	0.42 ± 0.33	0.47 ± 0.31	0.35 ± 0.31
ODE-LSTM (2020)	0.63 ± 0.24	0.57 ± 0.25	0.51 ± 0.24	0.45 ± 0.23
Neural SDE (2019)	0.48 ± 0.28	0.47 ± 0.26	0.45 ± 0.27	0.45 ± 0.25
Neural LNSDE (2024)	0.7 ± 0.27	0.68 ± 0.29	$\underline{0.67 \pm 0.25}$	$\mathbf{0.66 \pm 0.23}$
LDDMM (2008)	$\underline{0.72 \pm 0.2}$	$\underline{0.7 \pm 0.21}$	0.57 ± 0.25	0.4 ± 0.25
TS-LDDMM (ours)	$\mathbf{0.83 \pm 0.18}$	$\mathbf{0.8 \pm 0.18}$	$\mathbf{0.7 \pm 0.26}$	0.51 ± 0.27

I.5 Appendix for experiment: Classification benchmark on regularly sampled datasets

I.6 Settings

In this section, we compare classification performances of TS-LDDMM with other state-of-the-art methods coming from shape analysis on 15 shape-based datasets of time-series.

Methods We compare TS-LDDMM with a method from function [56]

	Dataset	Shape-FPCA (2024)	TCLR (2024)	LDDMM (2008)	TS-LDDMM (ours)
Univariate	ArrowHead	0.18	0.75	<u>0.84</u>	**0.91**
	BME	0.16	<u>1.00</u>	0.82	**1.00**
	ECG200	0.40	0.67	**0.81**	<u>0.79</u>
	FacesUCR	0.08	<u>0.73</u>	0.69	**0.86**
	GunPoint	0.93	<u>0.97</u>	0.83	**1.00**
	PhalangesOutlinesCorrect	0.39	**0.63**	<u>0.53</u>	0.52
	Trace	0.55	<u>1.00</u>	0.46	**1.00**
Multivariate	ArticularyWordRecognition	–	–	<u>0.98</u>	**1.00**
	Cricket	–	–	<u>0.77</u>	**0.93**
	ERing	–	–	<u>0.95</u>	**0.98**
	Handwriting	–	–	<u>0.22</u>	**0.44**
	Libras	–	–	<u>0.56</u>	**0.60**
	NATOPS	–	–	<u>0.82</u>	**0.82**
	RacketSports	–	–	**0.83**	<u>0.79</u>
	UWaveGestureLibrary	–	–	<u>0.72</u>	**0.81**

Protocole

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