
Shapes analysis for time series.

Anonymous Author(s)

Affiliation

Address

email

Abstract

1 Analyzing the inter-individual variability within a cluster of time series is particu-
2 larly appealing in medicine and biology. Individuals have specificities depending
3 on their genes or disease while sharing, on average, a similar pattern in the features
4 of their corresponding time series. For instance, an electrocardiogram presents
5 a typical shape of the heartbeat, which varies depending on the individual. This
6 paper introduces an unsupervised representation learning (URL) algorithm for time
7 series tailored to biomedical inter-individual studies. The idea is to represent time
8 series as the deformation of a time series of reference using Large Deformation
9 Diffeomorphic Metric Mapping (LDDMM). Once the deformations and time series
10 of reference are learned, the vector representations of time series are then given by
11 the parametrization of the deformation. At the crossroads between URL for time
12 series and shape analysis, the proposed algorithm manages irregularly sampled
13 multivariate time series of variable lengths and provides shape-based representa-
14 tions of temporal data. In this work, we establish a representation theorem for the
15 graph of a time series and derive its consequences on the LDDMM framework. We
16 showcase the advantages of our representation compared to existing methods using
17 synthetic data and real-world examples motivated by biomedical applications.

18 1 Introduction

19 Our goal is to analyze the inter-individual variability of a time series dataset, which is of prime
20 interest in medicine and biology [45, 3, 17]. More specifically, we aim to find an unsupervised
21 features representation method which encode the specificity of an individual compared to another. In
22 physiology, studying the different *shapes* in a time series related to biological phenomena and their
23 variations according to individual or pathology is common. However, a *shape* has no clear definition;
24 it is more an intuitive way to speak about the silhouette of a pattern in a time series. In this paper, we
25 refer to as the shape of a time series, the graph of this signal.

26 Although a community structure with representatives can be learned in an unsupervised way [43, 30]
27 using contrastive loss [16, 42, 30] or similarity measures [1, 17, 36, 48], studying the inter-individual
28 variability of shapes within a cluster [34, 40] is still an open problem in URL.

29 First, we propose not to see time series through their curve $\{s_t : t \in I\}$, but through their graph
30 $G(s) = \{(t, s(t)) : t \in I\}$. Then, building on the shape analysis literature [4, 44], we follow the
31 Large Deformation Diffeomorphic Metric Mapping (LDDMM) framework [4, 44] to analyze these
32 graphs. The idea is to represent each element $(G(s^j))_{j \in [N]}$ of the dataset as the transformation of a
33 reference graph $G(s_0)$ by a diffeomorphism. Then, the diffeomorphism is learned by integrating an
34 ordinary differential equation parameterized by a Reproducing Kernel Hilbert Space (RKHS). The
35 parameters $(\alpha_j)_{j \in [N]}$ encoding the diffeomorphisms $(\phi_j)_{j \in [N]}$ yield the representation features of the
36 graphs $(G(s^j))_{j \in [N]}$. Finally, these features encoding the shapes can feed any statistical or machine
37 learning model as in URL.

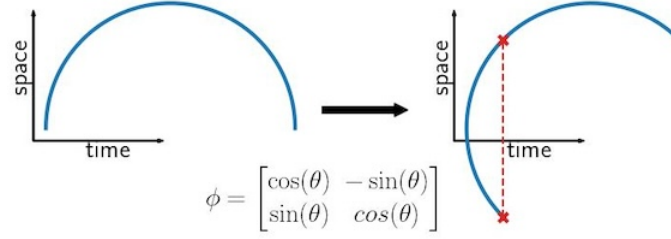


Figure 1: A time series’ graph $G = \{(t, s(t)) : t \in I\}$ can lose its structure after applying a general diffeomorphism ϕ . G : a time value can be related to two values on the space axis.

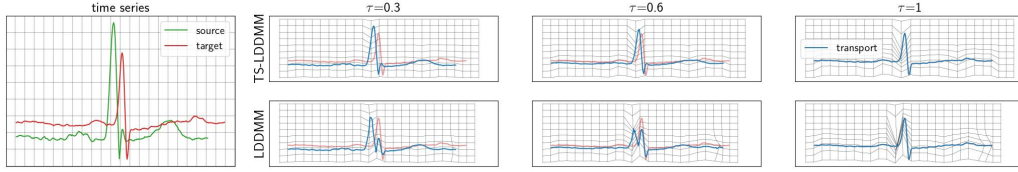


Figure 2: LDDMM and TS-LDDMM are applied to ECG data. We observe that LDDMM, using a general Gaussian kernel, does not learn the time translation of the first spike but changes the space values, i.e., one spike disappears before emerging at a translated position. At the same time, TS-LDDMM handles the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

38 However, a graph time series transformation by a general diffeomorphism is not always a graph time
 39 series, see e.g. Figure 1, thus a graph time series is more than a simple curve [19]. Our contributions
 40 arise from this observation. We solve this issue by specifying the class of diffeomorphisms to
 41 consider and showing how to learn them. This change is fruitful in representing time transformation
 42 as illustrated in Figure 2.

43 Our contributions can be summarized as follows:

- 44 • We propose an unsupervised method (TS-LDDMM) to analyze inter-individual variability
 45 of shapes in a time series dataset. In particular, the method can handle *irregularly sampled*
 46 time series with *variable sizes*.
- 47 • We motivate our extension of LDDMM to time series by introducing a theoretical framework
 48 with a representation theorem for time series graph (Theorem 1) and kernels related to their
 49 structure (Lemma 1).
- 50 • We demonstrate the identifiability of the model by estimating the true generating param-
 51 eter of synthetic data, and we highlight the sensitivity of our method with respect to its
 52 hyperparameters, also providing guidelines for tuning. We highlight the *interpretability* of
 53 TS-LDDMM for studying the inter-individual variability in a clinical dataset. We illustrate
 54 the quantitative interest of the representation on classification tasks on real shape-based
 55 datasets.

56 2 Related Works

57 Shape analysis focus on the statistical analysis of various mathematical objects invariant under
 58 rotations, dilations, or time parameterization. The main idea is to represent these different objects in
 59 a complete Riemannian manifold (\mathcal{M}, g) with a metric g adapted to the geometry of the problem
 60 [31]. Then, any set of points in \mathcal{M} can be represented as points in the tangent space of their Frechet
 61 mean m_0 [35, 27] by considering their logarithms. The goal is then to find a well suited Riemannian
 62 struvture according to the studied object.

A time series graph can be seen a curve and LDDMM structure is relevant to tackle curves as presented in [19]. However, time series graph has more structure as depicted in Figure 1 due to the temporal evolution. [37] tracks anatomical shape changes in serial images using LDDMM, but distinguish from us by including the temporal evolution at a higher level: the goal is to perform longitudinal data modeling.

Leaving the LDDMM representation, [41, 21] address the representation of curves having unitary velocity by using the Square-Root Velocity (SRV) representation. However, the SRV representation applies after a reparametrization in time, such that the original time evolution of the time series is not represented in the final features. Again, the time series graph structure is not respected. Very recently in a functional data analysis framework [46] (Shape-FPCA) improved by giving also a representation for the original time evolution. Nevertheless, this methods applies only on time series of *same size* and is made for *continuous objects*, making the estimation more sensitive to noise. [Ajouter littérature de URL demander à Sisi ?]

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 $C^m(I, E)$ the set of m -times continuously differentiable function defined on an open set U to a normed vector space E , by $\|u\|_\infty = \sup_{x \in U} |u(x)|$ for any bounded function $u : U \rightarrow E$, 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 diffeomorphisms 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 $\mathbb{R}^{d'}$, 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 diffeomorphisms as deformations. Such *deformations* ϕ are constructed via differential flow equations, for any $x_0 \in \mathbb{R}^{d'}$ and $\tau \in [0, 1]$:

$$\frac{dX(\tau)}{d\tau} = v_\tau(X(\tau)), \quad X(0) = x_0, \quad \phi_\tau^v(x_0) = X(\tau), \quad \phi^v = \phi_1^v, \quad (1)$$

where the velocity field is $v : \tau \in [0, 1] \mapsto v_\tau \in V$ and V is a Hilbert space of continuously differentiable function on $\mathbb{R}^{d'}$. If $\|du\|_\infty + \|u\|_\infty \leq \|u\|_V$ for any $u \in V$ and $v \in L^2([0, 1], V) = \{v \in C^0([0, 1], V) : \int_0^1 \|v_\tau\|_V^2 d\tau < \infty\}$, by [18, Theorem 5] ϕ^v exists and belongs to $\mathcal{D}(\mathbb{R}^{d'})$, where we denote by $\mathcal{D}(O)$ the set of diffeomorphism 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 $v \in L^2([0, 1], V) \mapsto \mathcal{L}(\phi^v \cdot \mathbf{x}, \mathbf{y})$, where \mathcal{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 $V_\Theta \subset L^2([0, 1], V)$, parameterized by Θ , which allows us to solve this minimization problem efficiently.

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

107 It has been proposed in [31] to interpret V as a tangent space relative to the group of diffeomorphisms
 108 $H = \{\phi^v : v \in L^2([0, 1], V)\}$. Following this geometric point of view, geodesics can be constructed
 109 on H by using the following squared norm

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

110 By deriving differential constraints related to the minimum of (2) and using Cauchy lipshcitz condi-
 111 tions, geodesics can be defined only by giving the starting point and the initial velocity $v_0 \in V$ [31],
 112 as straight lines in Euclidean space. Denoting by $w(v_0)$ the geodesic starting from the identity with
 113 initial velocity v_0 , the exponential map is defined as $\varphi^{\{v_0\}} \triangleq \phi^v$ and the previous matching problem
 114 becomes a *geodesic shooting problem*:

$$\inf_{v_0 \in V} \mathcal{L}(\varphi^{\{v_0\}} \cdot \mathbf{x}, \mathbf{y}). \quad (3)$$

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

118 **Discrete parametrization of diffeomorphism.** In this part, V is chosen as an RKHS [5] generated
 119 by a smooth kernel K (e.g., Gaussian). We follow [13] and define a discrete parameterization of the
 120 velocity fields to perform geodesics shooting (3). The initial velocity field v_0 is chosen as a finite
 121 linear combination of the RKHS basis vector fields, $\mathbf{X}_0 = (x_{k,0})_{k \in [\mathbf{n}_0]} \in (\mathbb{R}^{d'})^{\mathbf{n}_0}$
 122 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 $x \in \mathbb{R}^{d'}$,

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

123 In our applications, the control points $(x_{k,0})_{k \in [\mathbf{n}_0]}$ can be understood as the discretized graph
 124 $(t_k, \mathbf{s}_0(t_k))_{k \in [\mathbf{n}_0]}$ of a starting time series \mathbf{s}_0 . With this parametrization of v_0 , (author?) [31] show
 125 that the velocity field v of the solution of (3) keeps the same structure along time, such that for any
 126 $x \in \mathbb{R}^{d'}$ and $\tau \in [0, 1]$,

$$v_\tau(x) = \sum_{k=1}^{\mathbf{n}_0} K(x, x_k(\tau)) \alpha_k(\tau), \quad (5)$$

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

128 These equations are derived from the hamiltonian $H : (\alpha_k, x_k)_{k \in [\mathbf{n}_0]} \mapsto \sum_{k,l=1}^{\mathbf{n}_0} \alpha_k^\top K(x_k, x_l) \alpha_l$,
 129 such that the velocity norm is preserved $\|v_\tau\|_V = \|v_0\|_V$ for any $\tau \in [0, 1]$. By (5), the velocity
 130 field related to a geodesic v^* is fully parametrized by its initial control points and momentum
 131 $(x_{k,0}, \alpha_{k,0})_{k \in [\mathbf{n}_0]}$. Thus, given a set of targets $\mathbf{y} = (y_i)_{i \in [T_2]}$ in $\mathbb{R}^{d'}$, a set of starting points $\mathbf{x} =$
 132 $(x_{i,0})_{i \in [T_1]}$ in $\mathbb{R}^{d'}$, a RKHS's kernel $K : \mathbb{R}^{d'} \times \mathbb{R}^{d'} \rightarrow \mathbb{R}^{d' \times d'}$, a distance on sets \mathcal{L} , a numerical
 133 integration scheme of ODE and a penalty factor $\lambda > 0$, the basic geodesic shooting step minimizes
 134 the following function using a gradient descent method:

$$\mathcal{F}_{\mathbf{x}, \mathbf{y}} : (\alpha_k)_{k \in [T_1]} \mapsto \mathcal{L}(\varphi^{\{v_0\}} \cdot \mathbf{x}, \mathbf{y}) + \lambda \|v_0\|_V^2, \quad (6)$$

135 where v_0 is defined by (4) and $\varphi^{\{v_0\}} \cdot \mathbf{x}$ is the result of the numerical integration of (5) using control
 136 points \mathbf{x} and initial momentums $(\alpha_k)_{k \in [T_1]}$.

137 **Relation to Continuous Normalizing Flows.** One particular popular choice to address the problem
 138 of learning a diffeomorphism or a velocity field is Normalizing Flows [38, 26] (NF) or their continuous
 139 counterpart [9, 20, 39] (CNF). However, we do not rely on this class of learning algorithms for several
 140 reasons. Indeed, existing and simple normalizing flows are not suitable for the type of data that
 141 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 $j \in [N]$, $s^j \in C^1(I_j, \mathbb{R}^d)$. 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 necessary 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 $s : I \rightarrow \mathbb{R}^d$ is encoded in its graphs $G(s)$ defined as the set $\{(t, s(t)) : t \in I\}$ and not only in its values $s(I) = \{s(t) : t \in I\}$ 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 [47, 29].

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 [44], addressing similar problems in morphology, we suggest to represent each time series' graph $G(s^j)$ as the transformation of a reference graph $G(s_0)$, related to a time series $s_0 : I \rightarrow \mathbb{R}^d$, by a diffeomorphism ϕ_j on \mathbb{R}^{d+1} , for any $j \in [N]$,

$$\phi_j.G(s_0) = \{\phi_j(t, s_0(t)), t \in I\}. \quad (7)$$

s_0 will be understood as the typical representative shape common to the collection of time series $(s^j)_{j \in [N]}$. As 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 $G(s_0)$ 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 $G(s_0)$ as, for any $j \in [N]$,

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

with $\mathbf{n}_0 = \text{median}((n_j)_{j \in [N]})$, the representation problem given in (7) boils down solving:

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

which is carried out by a gradient descent on the control points \tilde{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{G}_0 is then considered as the \mathbf{n}_0 -samples of a common time series 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) ask to define a kernel and a loss in order to perform geodesic shooting 6, 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 $G(s)$ can result in a set $\phi.G(s)$ 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 $K : \mathbb{R}^{d+1} \times \mathbb{R}^{d+1} \rightarrow \mathbb{R}^{(d+1)^2}$ 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 \mathcal{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 $\Psi_\gamma \in \mathcal{D}(\mathbb{R}^{d+1}) : (t, x) \in \mathbb{R}^{d+1} \rightarrow (\gamma(t), x)$ for any $\gamma \in \mathcal{D}(\mathbb{R})$ and $\Phi_f : (t, x) \in \mathbb{R}^{d+1} \rightarrow (t, f(t, x))$ for any $f \in C^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$. We have the following representation theorem. All proofs are given in Appendix A.

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

Theorem 1. *Let $s : J \rightarrow \mathbb{R}^d$ and $s_0 : I \rightarrow \mathbb{R}^d$ be two continuously differentiable time series with I, J two intervals of \mathbb{R} . There exist $f \in C^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$ and $\gamma \in \mathcal{D}(\mathbb{R})$ such that $\gamma(I) = J$ and $\Phi_f \in \mathcal{D}(\mathbb{R}^{d+1})$,*

$$G(s) = \Pi_{\gamma, f}.G(s_0), \quad \Pi_{\gamma, f} = \Psi_\gamma \circ \Phi_f.$$

Moreover, for any $\bar{f} \in C^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$ and $\bar{\gamma} \in \mathcal{D}(\mathbb{R})$, there exists a continuously differentiable time series \bar{s} such that $G(\bar{s}) = \Pi_{\bar{\gamma}, \bar{f}}.G(s_0)$

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

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

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

$$K_G((t, x), (t', x')) = \begin{pmatrix} c_0 K_{\text{time}} & 0 \\ 0 & c_1 K_{\text{space}} \end{pmatrix}, \quad (9)$$

$$K_{\text{space}} = K_{\sigma_{T,1}}^{(1)}(t, t') K_{\sigma_x}^{(d)}(x, x') I_d, \quad K_{\text{time}} = K_{\sigma_{T,0}}^{(1)}(t, t'),$$

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 \mathbb{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 $\gamma \in \mathcal{D}(\mathbb{R})$ and $f \in C^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$ 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 $(\alpha_{k,0})_{k \in [n_0]} \in (\mathbb{R}^{d+1})^{n_0}$ 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 C, we give guidelines for selecting the hyperparameters $(\sigma_{T,0}, \sigma_{T,1}, \sigma_x, c_0, c_1)$.

226 **Loss** This section specifies the distance function \mathcal{L} introduced in the loss function defined in (6).

227 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
 228 potentially of different sizes n_j and sampled at different timestamps $(t_i^j)_{i \in [n_j]}$ for any $j \in [N]$. Usual
 229 metrics, such as the Euclidean distance, are not appealing as they make the underlying assumptions
 230 of equal size sets and the existence of a pairing between points. Distances between measures on sets
 231 (taking the empirical distribution), such as Maximum Mean Discrepancy (MMD) [14, 6], alleviate
 232 those issues; however, MMD only accounts for positional information and lacks information about
 233 the time evolution between sampled points. A classical data fidelity metric from shape analysis
 234 corresponding to the distance between *oriented varifolds* associated with curves alleviates this last
 235 issue [25]. Intuitively, an oriented varifold is a measure that accounts for positional and tangential
 236 information about the underlying curves at sample points. More details and information about
 237 *oriented varifolds* can be found in Appendix B.

238 More precisely, given two sets $G_0 = (g_i^0)_{i \in [T_0]}$, $G_1 = (g_i^1)_{i \in [T_1]} \in (\mathbb{R}^{d+1})^{T_1}$ and a kernel² $k :$
 239 $(\mathbb{R}^{d+1} \times \mathbb{S}^d)^2 \rightarrow \mathbb{R}$ verifying [25, Proposition 2 & 4], for any $\xi \in \{0, 1\}$ and $i \in [T_\xi - 1]$, denoting
 240 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
 241 $\vec{v}_i^\xi = (g_{i+1}^\xi - g_i^\xi)/l_i^\xi$, the varifold distance between G_0 and G_1 is defined as,

$$\begin{aligned} d_{W^*}^2(G_0, G_1) &= \sum_{i,j=1}^{T_0-1} l_i^0 k((c_i^0, \vec{v}_i^0), (c_j^0, \vec{v}_j^0)) l_j^0 - 2 \sum_{i=1}^{T_0-1} \sum_{j=1}^{T_1-1} l_i^0 k((c_i^0, \vec{v}_i^0), (c_j^1, \vec{v}_j^1)) l_j^1 \\ &\quad + \sum_{i,j=1}^{T_1-1} l_i^1 k((c_i^1, \vec{v}_i^1), (c_j^1, \vec{v}_j^1)) l_j^1 \end{aligned}$$

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

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

244 The specific kernels $k_{\text{pos}}, k_{\text{dir}}$ that we use in our experiments are given Appendix B.1. Note that
 245 the loss kernel k has nothing to do with the velocity field kernel denoted by K_G or K specified in
 246 Section 5.1. Finally, we define the data fidelity loss function, \mathcal{L} , as $d_{W^*}^2$, which is differentiable with
 247 regards to its first variable. For further readings on curves and surfaces representation as varifolds,
 248 readers can refer to [25, 8].

249 [Parler de méthode adaptatif ici](#)

250 6 Experiments

251 [L'intro est ce necessaire ?]

252 First, we show on synthetic data that the proposed representation is identifiable provided that the
 253 hyperparameters and the reference graph are wisely selected, i.e., the parameter v_0^* generating a
 254 deformation $\varphi^{\{v_0^*\}}$ of a time series graph G can be estimated from the data $G, \varphi^{\{v_0^*\}}.G$ by solving
 255 the geodesic shooting problem (6). Secondly, we illustrate the qualitative interest of TS-LDDMM in
 256 studying inter-individual variability on a clinical dataset. Thirdly, we demonstrate the quantitative
 257 performance of our representation by performing classification on shape-based datasets. The method
 258 is implemented on Python using the library JAX³. The code was compiled on a server with NVIDIA
 259 RTX A2000 12GB GPU, Intel(R) Xeon(R) Gold 5220R CPU @ 2.20GHz, and 250 GB of RAM. The
 260 code will be available on Github.

261 6.1 Synthetic experiments

262 First, we show the model identifiability when the kernel K_G is well specified: the estimated param-
 263 eter is a good approximation of the generating parameter when the generation and the estimation

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

³<https://github.com/google/jax>

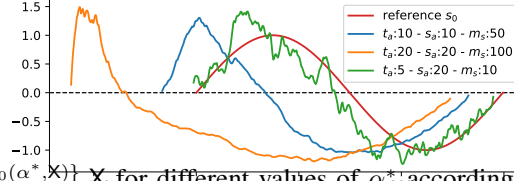


Figure 3: Plots of $\varphi^{\{v_0(\alpha^*, X)\}} \cdot X$ for different values of α^* according to its sampling parameter t_a, s_a, m_s , taking $X = G(s_0)$ with $s_0 : k \in [300] \rightarrow \sin(2\pi k/300)$.

Table 1: Values of $\mathcal{L}(\varphi^{\{v_0(\alpha^*, X)\}} \cdot X, \varphi^{\{\hat{v}_0\}} \cdot X)$ as α^* is sampled according to $\text{Gen}(10, 10, 50)$ 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

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 as $X = (x_k = (k, \sin(2\pi k/300)))_{k \in [300]}$. Given $m_s \in \mathbb{N}_{>0}$ and $t_a, s_a > 0$, we randomly generate initial momentums $\alpha^* = (\alpha_k^*)_{k \in [n_0]}$ with the following sampling, called $\text{Gen}(m_s, t_a, s_a)$: For any $k \in [n_0]$, α_k^* is sampled according to a Gaussian normal distribution $\mathcal{N}(0_{d+1}, I_{d+1})$. Then, $(\alpha_k^*)_{k \in [n_0]}$ is regularized by a rolling average of size m_s , we get $\bar{\alpha}' = (\bar{\alpha}'_k)_{k \in [n_0]}$. Finally, we normalize $\bar{\alpha}'$ to derive α^* such that $|([\alpha_k^*]_t)_{k \in [n_0]}| = t_{\text{amp}}$ and $|([\alpha_k^*]_s)_{k \in [n_0]}| = s_{\text{amp}}$ for any $k \in [n_0]$, denoting by $[\alpha_k^*]_t, [\alpha_k^*]_s$ the time and space coordinates of α_k^* respectively. Note that the regularizing step $(\alpha_k^*)_{k \in [n_0]} \rightarrow \bar{\alpha}'$ is necessary to obtain realistic deformations which take into account the regularity induced by the RKHS V . Then, using $v_0(\alpha^*, X)$ 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 $\varphi^{\{v_0\}} \cdot X$. Finally, we solve (6) to recover an estimation $\hat{\alpha}$ of α^* and report the average relative error (ARE) $|v_0(\hat{\alpha}, X) - v_0(\alpha^*, X)|_V / |v_0(\alpha^*, X)|_V$ 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 **0.10, 0.03, 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 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 $\mathcal{L}(\varphi^{\{v_0(\alpha^*, X)\}} \cdot X, \varphi^{\{\hat{v}_0\}} \cdot X)$ on 50 repetitions when α^* is sampled according to $\text{Gen}(10, 10, 50)$ and $\hat{v}_0 = v_0(\hat{\alpha}, X)$ denoting by $\hat{\alpha}$ the result of the minimization (6). 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 [33]. 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 airflow was recorded for 15 to 20 minutes before exposure to the irritant molecule and then for 35

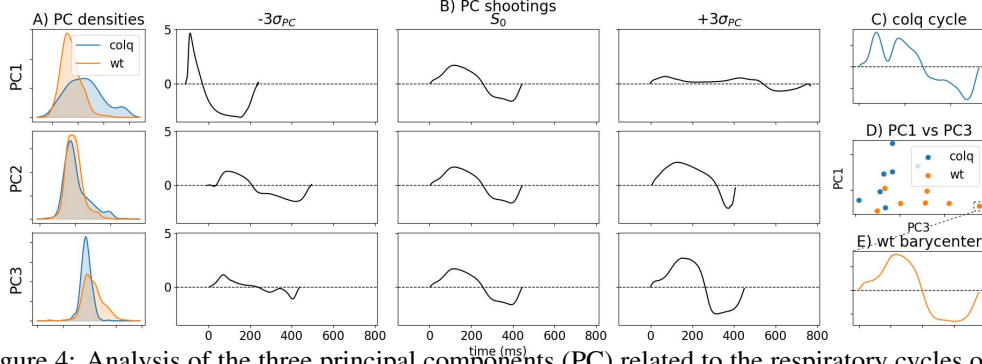


Figure 4: Analysis of the three principal components (PC) related to the respiratory cycles of the mouse before exposure. In Figure A), the densities of each genotype according to each PC are displayed. In Figure B), the deformations of the reference graph S_0 along each PC are given. In Figure D), the 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.

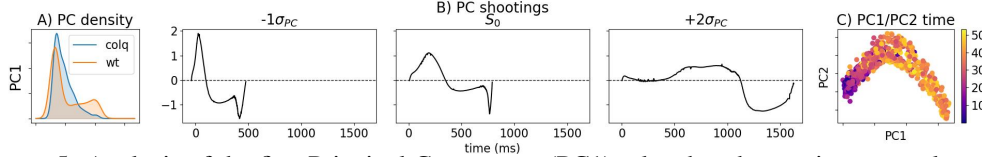


Figure 5: Analysis of the first Principal Component (PC1) related to the respiratory cycles of the mouse before and after exposure. In Figure A), the densities of each genotype according are displayed. In Figure B), the deformations of the reference graph S_0 PC1 is given. In Figure C), respiratory cycles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

302 to 40 minutes. A complete description of the dataset is given in the Appendix E. By comparing
 303 the shape of individual respiratory cycles (inspiration + expiration, see Figure 4-C)), we show that
 304 TS-LDDMM features can encode genotype distinctive breathing behaviors and their evolution after
 305 exposure to the irritant molecule.

306 We first compare breathing behaviors before exposure. Solving (8), we derive the reference respiratory
 307 cycle's graph S_0 and the TS-LDDMM features representations $(\alpha_j)_{j \in [N_1]}$ related to $N_1 = 700$
 308 respiratory cycles extracted according to the procedure [17]. Then, we perform a kernel PCA on the
 309 initial velocity field $(v_0(\alpha_j, S_0))_{j \in [N_1]} \in V^{N_1}$ defined in (4). In Figure 4, we focus on the analysis
 310 of the three Principal Components (PC).

311 As observable from Figure 4-B), principal components refer to different types of deformations. By
 312 interpreting Figure 4-B): Only PC1 accounts for time warping, PC2 expresses the trade-off between
 313 inspiration and expiration duration, and PC3 corresponds to a change in signal amplitude. Compared
 314 to **wt** mice, the distribution of **colq** mice TS-LDDMM feature representation along the PC1 axis
 315 has a heavy tail and the associated deformation ($+3 \sigma_{PC}$) shows an inspiration with two peaks. As
 316 illustrated in Figure 4-A), such respiratory cycles are preponderant with **colq** mice and may be caused
 317 by motor impairment due to their enzyme deficiency, [17]. In addition, the **colq** mice were smaller
 318 than the **wt** mice due to a delay in growth caused by their lack of an enzyme. This difference can be
 319 seen on PC3 since the volumes of air (area under the curve) inspired and exhaled are smaller for the
 320 smaller mice. In correlation, the distribution of **wt** mice TS-LDDMM feature representations along
 321 the PC3 axis have a heavy tail corresponding to large air volume as depicted by the deformation
 322 ($+3 \sigma_{PC}$) in Figure 4-B). Finally, Figure 4-D) shows that PC1 and PC3 capture the main differences
 323 between the two groups as their respective reference graphs S^j are located in different parts of the
 324 space.

325 We perform a second experiment to analyze the evolution of breathing behaviors when mice are
 326 exposed to the irritant molecule. We follow the same procedure as before. However, we take
 327 $N_2 = 1400$ with 25% (resp. 75%) before (resp. after) exposure. In Figure 5, we focus on the first
 328 principal component PC since it encodes the effect of the irritant molecule as depicted in Figure 5-C)
 329 (the exposure occurs at 20 minutes). Figure 5-B) shows that the deformation ($+3 \sigma_{PC}$) leads to

Table 2: Classification results in f1-score (U: unsupervised, S: supervised, DL: deep learning, ML: machine learning). \mathbf{x} best unsupervised method, \underline{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
DL	CNN	0.70	0.79	0.85	<u>0.96</u>
	ResNet	0.77	0.87	0.97	0.95
S	ML Catch22	0.73	0.81	0.96	0.89
	Rocket	<u>0.81</u>	<u>0.91</u>	<u>1.00</u>	0.88

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) [23], 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 [24]- and machine learning: Catch22 [28], Rocket [11], Dynamic Time Wrapping k-Nearest Neighbors (DTW-kNN) [32]. 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 results. 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.

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 relegated for future work.

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A Proofs

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

Theorem 4. Let $s : J \rightarrow \mathbb{R}^d$ and $s_0 : I \rightarrow \mathbb{R}^d$ be two continuously differentiable time series with I, J two intervals of \mathbb{R} . There exist $f \in C^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$ and $\gamma \in \mathcal{D}(\mathbb{R})$ such that $\gamma(I) = J$ and $\Phi_f \in \mathcal{D}(\mathbb{R}^{d+1})$,

$$G(s) = \Pi_{\gamma, f}.G(s_0), \quad \Pi_{\gamma, f} = \Psi_\gamma \circ \Phi_f.$$

Moreover, for any $\bar{f} \in C^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$ and $\bar{\gamma} \in \mathcal{D}(\mathbb{R})$, there exists a continuously differentiable time series \bar{s} such that $G(\bar{s}) = \Pi_{\bar{\gamma}, \bar{f}}.G(s_0)$

Proof. Let $s : J \rightarrow \mathbb{R}^d$ and $s_0 : I \rightarrow \mathbb{R}^d$ be two continuously differentiable time series with $I = (a, b)$, $J = (\alpha, \beta)$ 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 $\gamma(I) = J$ and $\gamma \in \mathcal{D}(\mathbb{R})$. By defining $f : (t, x) \in \mathbb{R}^{d+1} \mapsto x - s_0(t) + s \circ \gamma(t)$, the map $\Phi_f \in \mathcal{D}(\mathbb{R}^{d+1})$, indeed, its inverse is $\Phi_f^{-1} : (t, x) \in \mathbb{R}^{d+1} \mapsto (t, x + s_0(t) - s(t))$ and is continuously differentiable. Moreover, we have $\Pi_{\gamma, f}.G(s_0) = \{(\gamma(t), s \circ \gamma(t)) : t \in I\} = G(s)$.

Let $\bar{f} \in C^0(\mathbb{R}^{d+1}, \mathbb{R}^d)$, $\bar{\gamma} \in \mathcal{D}(\mathbb{R})$ and $s_0 \in C^0(I, \mathbb{R}^d)$ with I an interval of \mathbb{R} . We have :

$$\begin{aligned} \Pi_{\gamma, f}.G(s_0) &= \{(\gamma(t), f(t, s_0(t))), t \in I\} \\ &= \{(t, f(\gamma^{-1}(t), s_0(\gamma^{-1}(t)))) , t \in \gamma(I)\} . \end{aligned} \quad (10)$$

By defining $\bar{s} : t \in \gamma(I) \rightarrow f(\gamma^{-1}(t), s_0(\gamma^{-1}(t)))$, we have $\bar{s} \in C^0(\gamma(I), \mathbb{R}^d)$ by composition of continuous functions and $G(\bar{s}) = \Pi_{\gamma, f}.G(s_0)$ by (10), which concludes the proof. \square

Lemma 2. If we denote by \mathcal{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 $\gamma \in \mathcal{D}(\mathbb{R})$ and $f \in C^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$ 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 \mathcal{V} satisfying $\|f\|_{\mathcal{V}} \leq \|f\|_{\infty} + \|df\|_{\infty}$ for any $f \in \mathcal{V}$ 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 $C^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$, and by construction $\phi^v = \Psi_\gamma \circ \Phi_f$. \square

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 [25, 8]. We associate to $\gamma \in C^1((a, b), \mathbb{R}^{d+1})$ 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 $\omega : \mathbb{R}^{d+1} \times \mathbb{S}^d \rightarrow \mathbb{R}$,

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

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 $C^1((a, b), \mathbb{R}^{d+1})$ by the identification $\gamma \rightarrow \mu_\gamma$. Remark that in (TS-LDDMM), γ should be the parametrization of a time series' graph $G(s)$, i.e. $\gamma : t \in I \rightarrow (t, s(t)) \in \mathbb{R}^{d+1}$ denoting by $s : I \rightarrow \mathbb{R}^d$ 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 [25, Proposition 2 & 4] encourages us to consider a kernel $k : (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2 \rightarrow \mathbb{R}$ such that there exist two positive and continuously differentiable kernels k_{pos} and k_{dir} , such that for any $(x, \vec{u}), (y, \vec{v}) \in (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2$

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

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

Given such a kernel $k : (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2 \rightarrow \mathbb{R}$ verifying [25, Proposition 2 & 4], we have that for any $(x, v) \in \mathbb{R}^{d+1} \times \mathbb{S}^d$, $\delta_{(x, \vec{v})}$ belongs to W^* as a distribution and that the dual metric $\langle \cdot, \cdot \rangle_{W^*}$ satisfies for any $(x_1, v_1), (x_2, v_2) \in (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2$,

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

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

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

we have,

$$|\mu_X - \mu_Y|_{W^*}^2 = \sum_{i,j=1}^{T_0-1} l_i k((x_i, \vec{v}_i), (x_j, \vec{v}_j^0)) l_j - 2 \sum_{i=1}^{T_0-1} \sum_{j=1}^{T_1-1} l_i k((x_i, \vec{v}_i), (y_j, \vec{w}_j)) l'_j + \sum_{i,j=1}^{T_1-1} l'_i k((y_i, \vec{w}_i), (y_j, \vec{w}_j)) l'_j .$$

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

Now, we aim to discretize the oriented varifold μ_G related to a time series' graph $G(s)$ by using a set of triplets. This is carried out by using a discretized version of $G(s)$, i.e. $\tilde{G} = (g_i = (t_i, s(t_i)))_{i \in [T]} \in (\mathbb{R}^{d+1})^T$, in the following way: For any $i \in [T-1]$, denoting the center and length of the i^{th} segment

539 $[g_i, g_{i+1}]$ 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
540 $\vec{v}_i = (g_{i+1} - g_i)/l_i$, we define the set of triplets $X(\tilde{G}) = (l_i, c_i, \vec{v}_i)_{i \in [T-1]}$ and its related oriented
541 varifold $\mu_{X(\tilde{G})} = \sum_{i=1}^{T-1} l_i \delta_{c_i, \vec{v}_i}$ as in (11). This is a valid discretization of the oriented varifold μ_G
542 according to [25, Proposition 1]: $\mu_{X(\tilde{G})}$ converges towards μ_G as the size of the discretization mesh
543 $\sup_{i \in [T-1]} |t_{i+1} - t_i|$ converges to 0.

544 Finally, we define a distance on discretized time series' graphs \tilde{G}_1, \tilde{G}_2 as $d_{W^*}(\tilde{G}_1, \tilde{G}_2) =$
545 $d_{W^*,3}(X(\tilde{G}_1), X(\tilde{G}_2))$.

546 B.1 Varifold kernels

547 Denote the one-dimensional Gaussian kernel by $K_\sigma^{(a)}(x, y) = \exp(-|x - y|^2/\sigma)$ for any $(x, y) \in$
548 $(\mathbb{R}^a)^2$, $a \in \mathbb{N}$ and $\sigma > 0$. In the implementation, we use the following kernels, for any
549 $((t_1, x_1), (t_2, x_2)) \in (\mathbb{R}^{d+1})^2$, $((w_1, v_1), (w_2, v_2)) \in (\mathbb{S}^d)^2$,

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

550 where $\sigma_{\text{pos},t}, \sigma_{\text{pos},x}, \sigma_{\text{dir},t}, \sigma_{\text{dir},x} > 0$ are hyperparameters. In practice, we select $\sigma_{\text{pos},x} \approx \sigma_{\text{dir},x} \approx$
551 1 when the times series are centered and normalized. Otherwise we select $\sigma_{\text{pos},x} \approx \sigma_{\text{dir},x} \approx \bar{\sigma}_s$ with
552 $\bar{\sigma}_s$ the average standard deviation of the time series. We choose $\sigma_{\text{pos},t} \approx \sigma_{\text{dir},t} = m f_e$ with f_e the
553 sampling frequency of the time series and $m \in [5]$ an integer depending on the time change between
554 the starting and the target time series graph. The more significant the time change, the higher m
555 should be. The intuition comes from the fact that the width $\sigma_{\text{pos},t}, \sigma_{\text{dir},t}$ rules the time windows used
556 to perform the comparison, and $\sigma_{\text{pos},x}, \sigma_{\text{dir},x}$ affects the space window. The size of the windows
557 should be selected depending on the variations in the data.

558 C Tuning the hyperparameters of the TS-LDDMM kernel given in (9)

559 The parameter $\sigma_{T,0}$ should be chosen *large* compared the sampling frequency f_e and compared to
560 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
561 time transformation smoother. If $\sigma_{T,0}$ is too small, for instance, $\sigma_{T,0} = f_e$, the effect of the time
562 deformation is too localized, and there are not enough samples to make it visible.

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

566 We take $c_0 \approx 10c_1$, we want to encourage time transformation before space transformation. We take
567 $(c_0, c_1) = (1, 0.1)$ in all experiments.

568 D Numerical details

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

570 D.1 Optimization details of (8)

571 **Initialization** At the initialization of (8), all the momentums parameter are set to 0 and the graph of
572 reference is set to the graph of a time series in the dataset having a median samples size.

573 **Gradient descent.** The chosen gradient descent method is "adabelief" [49] implemented in the
574 library OPTAX⁴. There are two main parameters in the gradient descent: the number of steps nb_steps,
575 and the maximum value of step size η_M . The stepsize has a particular scheduling:

- 576 • Warmup period on $0.1 \times \text{nb_steps}$ steps: the stepsize increases linearly from 0 to η_M . The
577 goal is to learn progressively the parameters. If the stepsize is too large at the start, smaller
578 steps at the end can't make up for the mistakes made at the beginning.

⁴<https://optax.readthedocs.io/en/latest/>

579 • Fine tuning periode on $0.9 \times \text{nb_steps}$: the stepsize decreases from η_M to 0 with a cosine
580 decay implemented in the OPTAX scheduler, i.e. the decreasing factor as the form $0.5(1 +$
581 $\cos(\pi t/T))$.

582 The sharper the deformations, the larger the number of steps and the maximum value of step size
583 should be selected. We suggest $\text{nb_steps}=300$, $\eta_M = 0.1$ for small deformations and $\text{nb_steps}=800$,
584 $\eta_M = 0.3$ for big ones (time dilation with a factor $\lambda \geq 2$).

585 D.2 Synthetic experiments

586 For any deformations generation in both experiments (well-specified and misspecified), we take
587 $\sigma_{T,0}, \sigma_{T,1}, \sigma_x = (100, 1, 1)$ and $c_0, c_1 = (1, 0.1)$ for the kernel K_G and $\sigma_{\text{pos},t}, \sigma_{\text{pos},t}, \sigma_{\text{dir},t}, \sigma_{\text{dir},x} =$
588 $(2, 1, 2, 0.6)$ for the varifold kernels $k_{\text{pos}}, k_{\text{dir}}$ related to the loss \mathcal{L} .

589 In both experiments, we have $\text{nb_steps}=300$ and $\eta_M = 0.1$.

590 D.3 Mouse experiments

591 The number of steps is larger in the second experiment (before/after injection) because the deforma-
592 tions are sharper.

593 D.4 Classification experiments

594 We defined a default parametrization for all classifiers.

595 For classifiers: CNN, ResNet, Catch22, DTW-KNN, Rocket we used the aeon⁵ implementations with
596 their default settings.

597 For Tloss-SVC we used the implementation provided on github⁶ with the following parameters for
598 learning representations: batch_size: 10, channels: 40, depth: 10, nb_steps: 200, in_channels: 1, ker-
599 nel_size: 3, lr: 0.001, nb_random_samples: 10, negative_penalty: 1, out_channels: 320, reduced_size:
600 160. We used the Support Vector Classifier (SVC) from scikit-learn with the regularization term C:
601 1. Others parameters are set to default.

602 For TS-LDDMM-SVC, all kernels' parameters et optimizer parameter are presented in Table 3.
603 As well, we used the Support Vector Classifier from scikit-learn with the regularization term C: 1.
604 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	$(\text{nb_steps}, \eta_M)$	$(\sigma_{\text{pos},t}, \sigma_{\text{pos},t}, \sigma_{\text{dir},t}, \sigma_{\text{dir},x})$	$(c_0, c_1, \sigma_{T,0}, \sigma_{T,1}, \sigma_x)$
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)	$(\max(2, 0.03\bar{l}), N_d, \max(2, 0.03\bar{l}), 0.6)$	$(1, 0.1, 0.33\bar{l}, 1, N_d)$

605 E Mouse respiratory dataset

606 Ventilation is a simple physiological function that ensures a vital supply of oxygen and the elimination
607 of CO2. Acetylcholine (Ach) is a neurotransmitter that plays an important role in muscular activity,
608 notably for breathing. Indeed, muscle contraction information passes from the brain to the muscle

⁵<https://www.aeon-toolkit.org/en/stable/index.html>

⁶<https://github.com/mqwfrog/ULTS>

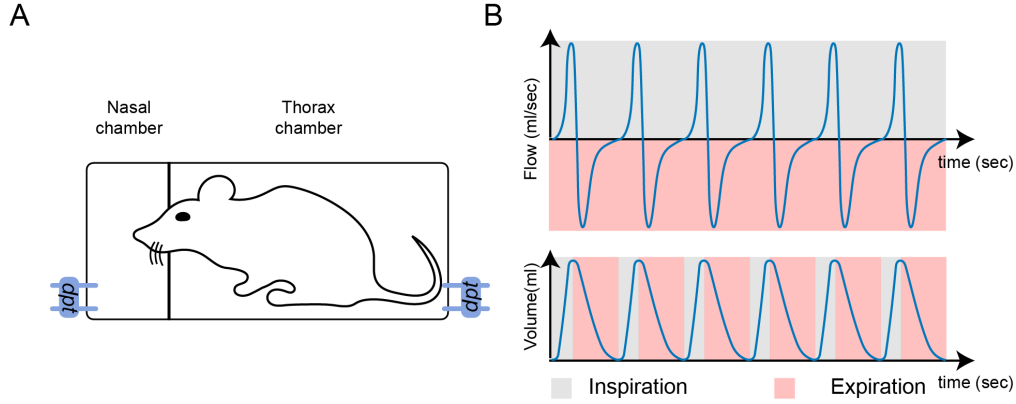


Figure 6: A: Illustration of a double-chamber plethysmograph. The term *dpt* stands for differential pressure transducer which measures the pressure in each compartment, the pressure then being converted to flow. B: Nasal airflow (top) and lung volume (bottom). During inspiration, airflow is positive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

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 [33], 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 [22], 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 [33], 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 datasets⁷, 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.

⁷<https://timeseriesclassification.com>

⁸<https://www.aeon-toolkit.org/en/stable/>

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

Dataset	Train size	test size	Length	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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