
Shapes analysis for time series.

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Abstract

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

15 1 Introduction

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

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

26 First, we propose not to see time series through their curve $\{s_t : t \in I\}$, but through their graph
27 $G(s) = \{(t, s(t)) : t \in I\}$. Then, building on the shape analysis literature [4, 41], we follow the
28 Large Deformation Diffeomorphic Metric Mapping (LDDMM) framework [4, 41] to analyze these
29 graphs. The idea is to represent each element $(G(s^j))_{j \in [N]}$ of the dataset as the transformation of a
30 reference graph $G(s_0)$ by a diffeomorphism. Then, the diffeomorphism is learned by integrating an
31 ordinary differential equation parameterized by a Reproducing Kernel Hilbert Space (RKHS). The
32 parameters $(\alpha_j)_{j \in [N]}$ encoding the diffeomorphisms $(\phi_j)_{j \in [N]}$ yield the representation features of the
33 graphs $(G(s^j))_{j \in [N]}$. Finally, these features encoding the shapes can feed any statistical or machine
34 learning model as in URL.

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

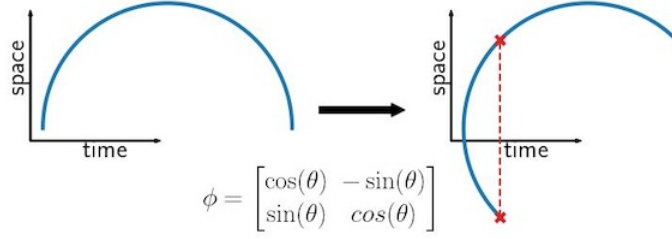


Figure 1: A time series’ graph $G = \{(t, s(t)) : t \in I\}$ can lose its structure after applying a general diffeomorphism ϕ . G : a time value can be related to two values on the space axis.

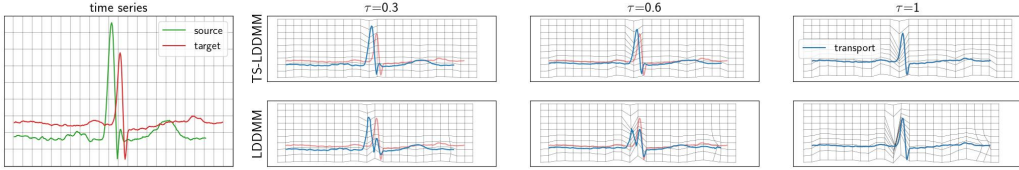


Figure 2: LDDMM and TS-LDDMM are applied to ECG data. We observe that LDDMM, using a general Gaussian kernel, does not learn the time translation of the first spike but changes the space values, i.e., one spike disappears before emerging at a translated position. At the same time, TS-LDDMM handles the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

38 consider and showing how to learn them. This change is fruitful in representing time transformation
 39 as illustrated in Figure 2.

40 Our contributions can be summarized as follows:

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

53 2 Related Works

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

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

61 3 Notations

62 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
 63 $C^m(I, E)$ the set of m -times continuously differentiable function defined on an open set U to a normed
 64 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
 65 set of positive integers.

66 4 Background on LDDMM

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

71 In the next section, the time series are going to be represented by diffeomorphism parameters
 72 $(\alpha_j)_{j \in [N]}$. That's why LDDMM is chosen since it offers a parametrization for diffeomorphisms which
 73 is sparse and interpretable, two features particularly relevant in the biomedical context.

74 The basic problem that we consider in this section is the following. Given a set of targets $\mathbf{y} =$
 75 $(y_i)_{i \in [T_2]}$ 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
 76 such that the finite set of points \mathbf{y} is similar in a certain sense to the set of finite sets of transformed
 77 points $\phi \cdot \mathbf{x} = (\phi(x_i))_{i \in [T_1]}$. The function ϕ is occasionally referred to as a *deformation*. In general,
 78 these sets \mathbf{x}, \mathbf{y} are meshes of continuous objects, e.g surfaces, curves, images and so on.

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

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

81 where the velocity field is $v : \tau \in [0, 1] \mapsto v_\tau \in V$ and V is a Hilbert space of continuously
 82 differentiable function on $\mathbb{R}^{d'}$. If $\|du\|_\infty + \|u\|_\infty \leq \|u\|_V$ for any $u \in V$ and $v \in L^2([0, 1], V) =$
 83 $\{v \in C^0([0, 1], V) : \int_0^1 \|v_\tau\|_V^2 d\tau < \infty\}$, by [18, Theorem 5] ϕ^v exists and belongs to $\mathcal{D}(\mathbb{R}^{d'})$, where
 84 we denote by $\mathcal{D}(O)$ the set of diffeomorphism defined on an open set O to O . Therefore, for any
 85 choice of v , ϕ^v defines a valid deformation. This offers a general recipe to construct diffeomorphism
 86 given a functional space V .

87 With this in mind, the velocity field v fitting the data can be estimated by minimizing $v \in$
 88 $L^2([0, 1], V) \mapsto \mathcal{L}(\phi^v \cdot \mathbf{x}, \mathbf{y})$, where \mathcal{L} is an appropriate loss function. However, two computa-
 89 tional challenges arise. First, this optimization problem is ill-posed, and a penalty term is needed
 90 to obtain a unique solution. In addition, we have to find a parametric family $V_\Theta \subset L^2([0, 1], V)$,
 91 parameterized by Θ , which allows us to solve this minimization problem efficiently.

92 It has been proposed in [30] to interpret V as a tangent space relative to the group of diffeomorphisms
 93 $H = \{\phi^v : v \in L^2([0, 1], V)\}$. Following this geometric point of view, geodesics can be constructed
 94 on H by using the following squared norm

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

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

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

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

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

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

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

108 In our applications, the control points $(x_{k,0})_{k \in [\mathbf{n}_0]}$ can be understood as the discretized graph
 109 $(t_k, s_0(t_k))_{k \in [\mathbf{n}_0]}$ of a starting time series s_0 . With this parametrization of v_0 , (author?) [30] show
 110 that the velocity field v of the solution of (3) keeps the same structure along time, such that for any
 111 $x \in \mathbb{R}^{d'}$ and $\tau \in [0, 1]$,

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

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

112 These equations are derived from the hamiltonian $H : (\alpha_k, x_k)_{k \in [\mathbf{n}_0]} \mapsto \sum_{k,l=1}^{\mathbf{n}_0} \alpha_k^\top K(x_k, x_l) \alpha_l$,
 113 such that the velocity norm is preserved $\|v_\tau\|_V = \|v_0\|_V$ for any $\tau \in [0, 1]$. By (5), the velocity
 114 field related to a geodesic v^* is fully parametrized by its initial control points and momentum
 115 $(x_{k,0}, \alpha_{k,0})_{k \in [\mathbf{n}_0]}$. Thus, given a set of targets $\mathbf{y} = (y_i)_{i \in [T_2]}$ in $\mathbb{R}^{d'}$, a set of starting points $\mathbf{x} =$
 116 $(x_{i,0})_{i \in [T_1]}$ 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
 117 integration scheme of ODE and a penalty factor $\lambda > 0$, the basic geodesic shooting step minimizes
 118 the following function using a gradient descent method:

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

120 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
 121 points \mathbf{x} and initial momentums $(\alpha_k)_{k \in [T_1]}$.

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

133 5 Methodology

134 We consider in this paper observations which consist in a population of N multivariate time series, for
 135 any $j \in [N]$, $s^j \in C^1(I_j, \mathbb{R}^d)$. However, we can only access a n_j -samples $\tilde{s}^j = (\tilde{s}_i^j = s^j(t_i^j))_{i \in [n_j]}$
 136 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**
 137 **necessary the same accross individuals** and the timestamps can be **irregularly sampled**. We assume
 138 the time series population is globally homogeneous regarding their "shapes" even if inter-individual
 139 variability exists. Intuitively speaking, the "shape" of a time series $s : I \rightarrow \mathbb{R}^d$ is encoded in its graphs
 140 $G(s)$ 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
 141 time axis is crucial. As a motivating use-case, s^j can be the time series of a heartbeat extracted from
 142 an individual's electrocardiogram (ECG), see Figure 2. The homogeneity in a resulting dataset comes
 143 from the fact that humans have similar shapes of heartbeat [43, 28].

The deformation problem. In this paper, we aim to study the inter-individual variability in the dataset by finding a relevant representation of each time series. Inspired from the framework of shape analysis [41], addressing similar problems in morphology, we suggest to represent each time series' graph $G(s^j)$ 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 $j \in [N]$,

$$\mathbf{y}_j = G(\tilde{s}^j) = (t_i^j, \tilde{s}_i^j)_{i \in [n_j]} \in (\mathbb{R}^{d+1})^{n_j}, \quad \tilde{G}_0 = (t_i^0, \tilde{s}_i^0)_{i \in [n_0]} \in (\mathbb{R}^{d+1})^{n_0},$$

with $n_0 = \text{median}((n_j)_{j \in [N]})$, the representation problem given in (7) boils down solving:

$$\text{argmin}_{\tilde{G}_0, (\alpha_k^j)_{k \in [n_0]}} \sum_{j=1}^N \mathcal{F}_{\tilde{G}_0, \mathbf{y}_j} \left((\alpha_k^j)_{k \in [n_0]} \right), \quad (8)$$

which is carried out by a gradient descent on the control points \tilde{G}_0 and the momentums $\alpha_j = (\alpha_k^j)_{k \in [n_0]}$ for any $j \in [N]$, initialized by a dataset's time series graph of size n_0 and by $0_{(d+1)n_0}$ respectively. The optimization hyperparameter details are given in Appendix D.1. The result of the minimization \tilde{G}_0 is then considered as the 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}^{dn_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 $s : \mathbb{J} \rightarrow \mathbb{R}^d$ and $s_0 : \mathbb{I} \rightarrow \mathbb{R}^d$ be two continuously differentiable time series with \mathbb{I}, \mathbb{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 $\gamma(\mathbb{I}) = \mathbb{J}$ and $\Phi_f \in \mathcal{D}(\mathbb{R}^{d+1})$,

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

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 $G(\bar{s}) = \Pi_{\bar{\gamma}, \bar{f}} \cdot G(s_0)$

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

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

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 $(\alpha_{k,0})_{k \in [\mathbf{n}_0]} \in (\mathbb{R}^{d+1})^{\mathbf{n}_0}$ 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 C, we give guidelines for selecting the hyperparameters $(\sigma_{T,0}, \sigma_{T,1}, \sigma_x, c_0, c_1)$.

Loss This section specifies the distance function \mathcal{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 Discrepancy (MMD) [14, 6], alleviate those issues; however, MMD only accounts for positional information and lacks information about the time evolution between sampled points. A classical data fidelity metric from shape analysis corresponding to the distance between *oriented varifolds* associated with curves alleviates this last issue [24]. Intuitively, an oriented varifold is a measure that accounts for positional and tangential information about the underlying curves at sample points. More details and information about *oriented varifolds* can be found in Appendix B.

More precisely, given two sets $G_0 = (g_i^0)_{i \in [T_0]}, G_1 = (g_i^1)_{i \in [T_1]} \in (\mathbb{R}^{d+1})^{T_1}$ and a kernel² $k : (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2 \rightarrow \mathbb{R}$ verifying [24, Proposition 2 & 4], for any $\xi \in \{0, 1\}$ and $i \in [T_\xi - 1]$, denoting the center and length of the i^{th} segment $[g_i^\xi, g_{i+1}^\xi]$ by $c_i^\xi = (g_i^\xi + g_{i+1}^\xi)/2$, $l_i^\xi = \|g_{i+1}^\xi - g_i^\xi\|$, and

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

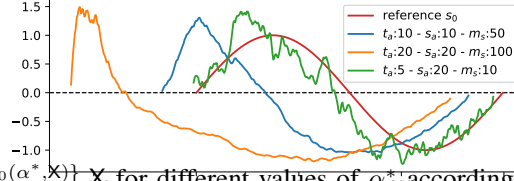


Figure 3: Plots of $\varphi^{v_0(\alpha^*, X)}$ for different values of α^* according to its sampling parameter t_a, s_a, m_s , taking $X = G(s_0)$ with $s_0 : k \in [300] \rightarrow \sin(2\pi k/300)$.

Table 1: Values of $\mathcal{L}(\varphi^{v_0(\alpha^*, X)}, X, \varphi^{\hat{v}_0}, X)$ 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

226 $\vec{v}_i^\xi = (g_{i+1}^\xi - g_i^\xi)/l_i^\xi$, the varifold distance between G_0 and G_1 is defined as,

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

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

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

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

234 [Parler de méthode adaptatif ici](#)

235 6 Experiments

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

245 6.1 Synthetic experiments

246 First, we show the model identifiability when the kernel K_G is well specified: the estimated param-
247 eter is a good approximation of the generating parameter when the generation and the estimation
248 procedure use the same hyperparameters for the RKHS kernel K_G . All the hyperparameter val-
249 ues for generation and estimation are given in Appendix D.2. We fix the initial control points

³<https://github.com/google/jax>

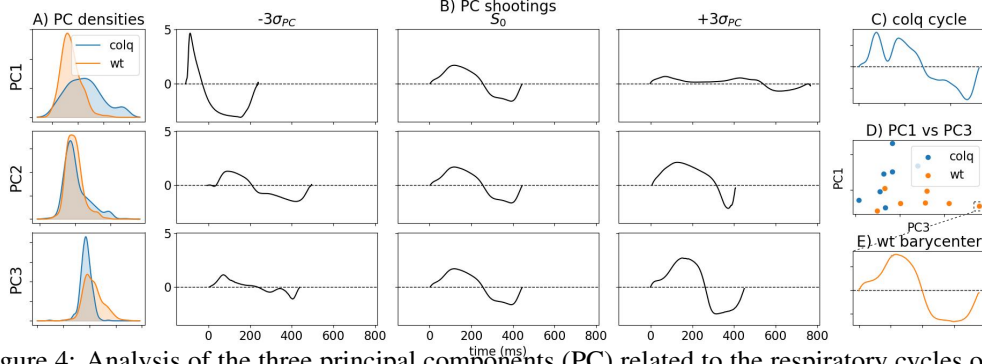


Figure 4: Analysis of the three principal components (PC) related to the respiratory cycles of the mouse before exposure. In Figure A), the densities of each genotype according to each PC are displayed. In Figure B), the deformations of the reference graph S_0 along each PC are given. In Figure D), the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

as $\mathbf{X} = (x_k = (k, \sin(2\pi k/300)))_{k \in [300]}$. 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 $\text{Gen}(m_s, t_a, s_a)$: 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 $(\alpha_k')_{k \in [\mathbf{n}_0]} \rightarrow \bar{\alpha}'$ is necessary to obtain realistic deformations which take into account the regularity induced by the RKHS \mathbf{V} . Then, using $v_0(\alpha^*, \mathbf{X})$ as defined in (4) with initial momentums α^* and control points \mathbf{X} , we apply the induced deformation $\varphi^{\{v_0\}}$ by (5) to \mathbf{X} and obtain $\varphi^{\{v_0\}} \cdot \mathbf{X}$. Finally, we solve (6) to recover an estimation $\hat{\alpha}$ of α^* and report the average relative error (ARE) $|v_0(\hat{\alpha}, \mathbf{X}) - v_0(\alpha^*, \mathbf{X})|_{\mathbf{V}} / |v_0(\alpha^*, \mathbf{X})|_{\mathbf{V}}$ 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 $\mathcal{L}(\varphi^{\{v_0(\alpha^*, \mathbf{X})\}} \cdot \mathbf{X}, \varphi^{\{v_0\}} \cdot \mathbf{X})$ on 50 repetitions when α^* is sampled according to $\text{Gen}(10, 10, 50)$ and $\hat{v}_0 = v_0(\hat{\alpha}, \mathbf{X})$ 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 [32]. The dataset is divided into two groups, one composed of 7 control mice (**wt**) and the other of 7 mice (**colq**) deficient in an enzyme involved in the control of respiration. For each mouse, the respiratory

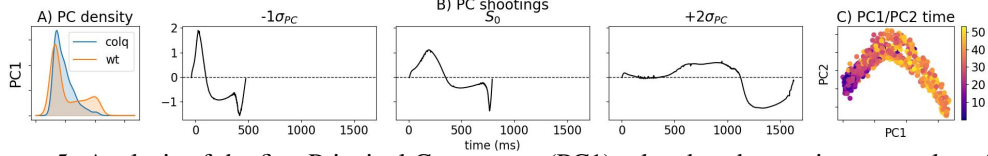


Figure 5: Analysis of the first Principal Component (PC1) related to the respiratory cycles of the mouse before and after exposure. In Figure A), the densities of each genotype according are displayed. In Figure B), the deformations of the reference graph S_0 PC1 is given. In Figure C), respiratory cycles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

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

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

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

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

6.3 Quantitative performances of the TS-LDDMM representation in classification

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

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

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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460 A Proofs

461 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 $G(s)$.

463 **Theorem 4.** *Let $s : J \rightarrow \mathbb{R}^d$ and $s_0 : I \rightarrow \mathbb{R}^d$ be two continuously differentiable time series*
 464 *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*
 465 $\Phi_f \in \mathcal{D}(\mathbb{R}^{d+1})$,

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

466 *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*
 467 *series \bar{s} such that $G(\bar{s}) = \Pi_{\bar{\gamma}, \bar{f}}.G(s_0)$*

468 *Proof.* Let $s : J \rightarrow \mathbb{R}^d$ and $s_0 : I \rightarrow \mathbb{R}^d$ be two continuously differentiable time series with
 469 $I = (a, b)$, $J = (\alpha, \beta)$ two intervals of \mathbb{R} . By setting $\gamma : t \in \mathbb{R} \mapsto (\beta - \alpha)(t - a)/(b - a) + \alpha \in \mathbb{R}$,
 470 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
 471 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
 472 continuously differentiable. Moreover, we have $\Pi_{\gamma, f}.G(s_0) = \{(\gamma(t), s \circ \gamma(t)) : t \in I\} = G(s)$.

473 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 :

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

474 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
 475 continuous functions and $G(\bar{s}) = \Pi_{\gamma, f}.G(s_0)$ by (10), which concludes the proof. \square

476 **Lemma 2.** *If we denote by V the RKHS associated with the kernel K_G , then for any vector field*
 477 *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*
 478 $\phi^v = \Psi_\gamma \circ \Phi_f$.

479 *Proof.* Let v be a vector field generated by (5) with v_0 satisfying (4). We remark that the first
 480 coordinate of the velocity field v_τ denoted by v_τ^{time} only depends on the time variable t for any
 481 $\tau \in [0, 1]$. Thus, when computing the first coordinate of the deformation ϕ^v , denoted by γ , we
 482 integrate (1) with v_τ replaced by v_τ^{time} , thus γ is independant of the variable x . Moreover, $\gamma \in \mathcal{D}(\mathbb{R})$
 483 since a Gaussian kernel induced an Hilbert space V satisfying $|f|_V \leq |f|_\infty + |df|_\infty$ for any $f \in V$
 484 by [18, Theorem 9]. For the same reason, we have $\phi^v \in \mathcal{D}(\mathbb{R}^{d+1})$, and thus its last coordinates
 485 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

486 B Oriented varifold

487 In this section, we introduce the *oriented varifold* associated with curves. For further readings
 488 on curves and surfaces representation as varifolds, readers can refer to [24, 8]. We associate to
 489 $\gamma \in C^1((a, b), \mathbb{R}^{d+1})$ an *oriented varifold* μ_γ , i.e. a distribution on the space $\mathbb{R}^{d+1} \times \mathbb{S}^d$ defined as
 490 follows, for any smooth test function $\omega : \mathbb{R}^{d+1} \times \mathbb{S}^d \rightarrow \mathbb{R}$,

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

491 Denoting by W the space of smooth test function, we have that μ_γ belongs to its dual W^* . Thus,
 492 a distance on W^* is sufficient to set a distance on oriented varifolds associated to curve and thus
 493 on $C^1((a, b), \mathbb{R}^{d+1})$ by the identification $\gamma \rightarrow \mu_\gamma$. Remark that in (TS-LDDMM), γ should be
 494 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
 495 $s : I \rightarrow \mathbb{R}^d$ the time series. However, in practice, we work with discrete objects. That is why, we
 496 set W as an RKHS to use its representation theorem. More specifically [24, Proposition 2 & 4]
 497 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
 498 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 [24, 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,

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

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 $[g_i, g_{i+1}]$ by $c_i = (g_i + g_{i+1})/2$, $l_i = \|g_{i+1} - g_i\|$, and the unit norm vector of direction $\vec{g_i g_{i+1}}$ by $\vec{v}_i = (g_{i+1} - g_i)/l_i$, we define the set of triplets $X(\tilde{G}) = (l_i, c_i, \vec{v}_i)_{i \in [T-1]}$ and its related oriented 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 according to [24, Proposition 1]: $\mu_{X(\tilde{G})}$ converges towards μ_G as the size of the discretization 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{G}_1, \tilde{G}_2 as $d_{W^*}(\tilde{G}_1, \tilde{G}_2) = d_{W^*,3}(X(\tilde{G}_1), X(\tilde{G}_2))$.

B.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 $((t_1, x_1), (t_2, x_2)) \in (\mathbb{R}^{d+1})^2, ((w_1, v_1), (w_2, v_2)) \in (\mathbb{S}^d)^2$,

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

where $\sigma_{\text{pos},t}, \sigma_{\text{pos},x}, \sigma_{\text{dir},t}, \sigma_{\text{dir},x} > 0$ are hyperparameters. In practice, we select $\sigma_{\text{pos},x} \approx \sigma_{\text{dir},x} \approx 1$ 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 $\bar{\sigma}_s$ 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 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 $\sigma_{\text{pos},t}, \sigma_{\text{dir},t}$ rules the time windows used to perform the comparison, and $\sigma_{\text{pos},x}, \sigma_{\text{dir},x}$ affects the space window. The size of the windows should be selected depending on the variations in the data.

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

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.

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

539 We take $c_0 \approx 10c_1$, we want to encourage time transformation before space transformation. We take
540 $(c_0, c_1) = (1, 0.1)$ in all experiments.

541 D Numerical details

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

543 D.1 Optimization details of (8)

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

546 **Gradient descent.** The chosen gradient descent method is "adabelief" [45] implemented in the
547 library OPTAX⁴. There are two main parameters in the gradient descent: the number of steps nb_steps,
548 and the maximum value of step size η_M . The stepsize has a particular scheduling:

- 549 • Warmup period on $0.1 \times \text{nb_steps}$ steps: the stepsize increases linearly from 0 to η_M . The
550 goal is to learn progressively the parameters. If the stepsize is too large at the start, smaller
551 steps at the end can't make up for the mistakes made at the beginning.
- 552 • Fine tuning periode on $0.9 \times \text{nb_steps}$: the stepsize decreases from η_M to 0 with a cosine
553 decay implemented in the OPTAX scheduler, i.e. the decreasing factor as the form $0.5(1 +$
554 $\cos(\pi t/T))$.

555 The sharper the deformations, the larger the number of steps and the maximum value of step size
556 should be selected. We suggest nb_steps=300, $\eta_M = 0.1$ for small deformations and nb_steps=800,
557 $\eta_M = 0.3$ for big ones (time dilation with a factor $\lambda \geq 2$).

558 D.2 Synthetic experiments

559 For any deformations generation in both experiments (well-specified and misspecified), we take
560 $\sigma_{T,0}, \sigma_{T,1}, \sigma_x = (100, 1, 1)$ and $c_0, c_1 = (1, 0.1)$ for the kernel K_G and $\sigma_{\text{pos},t}, \sigma_{\text{pos},t}, \sigma_{\text{dir},t}, \sigma_{\text{dir},x} =$
561 $(2, 1, 2, 0.6)$ for the varifold kernels $k_{\text{pos}}, k_{\text{dir}}$ related to the loss \mathcal{L} .

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

563 D.3 Mouse experiments

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

566 D.4 Classification experiments

567 We defined a default parametrization for all classifiers.

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

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

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

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

⁶<https://github.com/mqwfrog/ULTS>

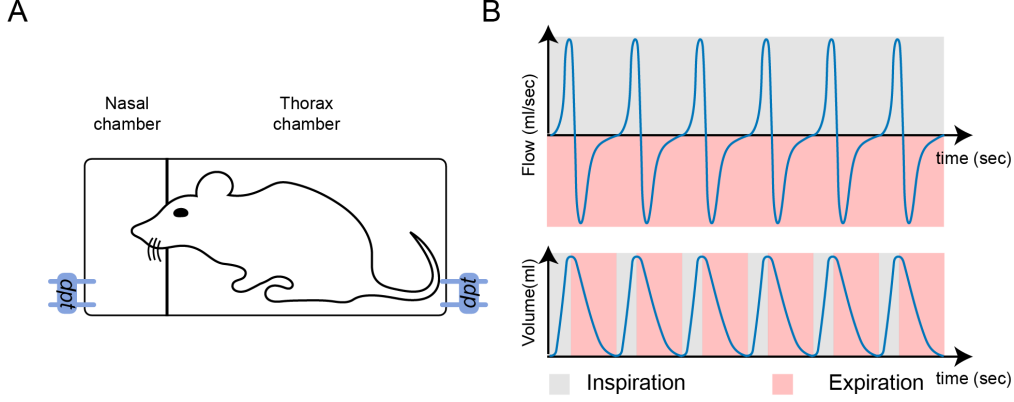


Figure 6: A: Illustration of a double-chamber plethysmograph. The term *dpt* stands for differential pressure transducer which measures the pressure in each compartment, the pressure then being converted to flow. B: Nasal airflow (top) and lung volume (bottom). During inspiration, airflow is positive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

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

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

objects	Optimizer	$k_{\text{pos}}, k_{\text{dir}}$	K_G
Parameter	$(\text{nb_steps}, \eta_M)$	$(\sigma_{\text{pos},t}, \sigma_{\text{pos},t}, \sigma_{\text{dir},t}, \sigma_{\text{dir},x})$	$(c_0, c_1, \sigma_{T,0}, \sigma_{T,1}, \sigma_x)$
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)	$(\max(2, 0.03\bar{l}), N_d, \max(2, 0.03\bar{l}), 0.6)$	$(1, 0.1, 0.33\bar{l}, 1, N_d)$

E Mouse respiratory dataset

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

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

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

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

F Classification datasets

All datasets were taken from UCR/UEA archives [10, 2]. Among all available 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.

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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⁷<https://timeseriesclassification.com>

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

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