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# Shapes analysis for time series.

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## Abstract

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

## 1 Introduction

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

25 Although community structures with representatives can be learned in an unsupervised manner  
26 [52, 37] using contrastive loss [18, 51, 37] or similarity measures [2, 19, 43, 58], the study of inter-  
27 individual variability of shapes within a cluster [40, 48] remains an open problem in unsupervised  
28 representation learning (URL), particularly for *irregularly sampled* time series with *variable lengths*.  
29

30 Our work explicitly focuses on learning shape-based representation of time series. First, we propose  
31 to view the shape of a time series not merely as its curve  $\{s_t : t \in I\}$ , but as its graph  $G(s) =$   
32  $\{(t, s(t)) : t \in I\}$ . Then, building on the shape analysis literature [5, 54], we adopt the Large  
33 Deformation Diffeomorphic Metric Mapping (LDDMM) framework [5, 54] to analyze these graphs.  
34 The core idea is to represent each element  $G(s^j)$  of a dataset  $(s^j)_{j \in [N]}$  as the transformation of a  
35 reference graph  $G(s_0)$  by a diffeomorphism  $\phi_j$ , i.e.  $G(s^j) \sim \phi_j.G(s_0)$ . The diffeomorphism  $\phi_j$   
36 is learned by integrating an ordinary differential equation parameterized by a Reproducing Kernel  
37 Hilbert Space (RKHS). The parameters  $(\alpha_j)_{j \in [N]}$  encoding the diffeomorphisms  $(\phi_j)_{j \in [N]}$  yield the

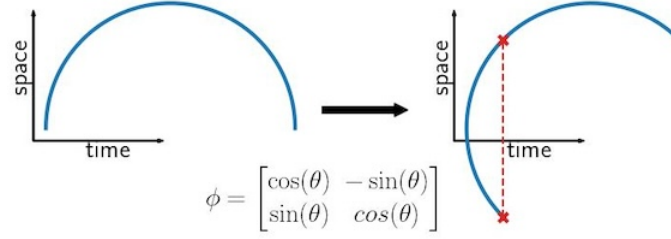


Figure 1: A time series' graph  $G = \{(t, s(t)) : t \in I\}$  can lose its structure after applying a general diffeomorphism  $\phi$ .  $G$ : a time value can be related to two values on the space axis.

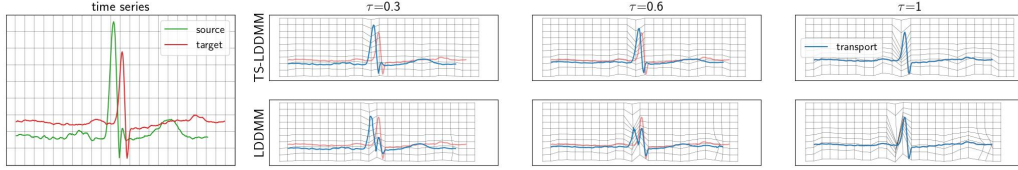


Figure 2: LDDMM and TS-LDDMM are applied to ECG data. We observe that LDDMM, using a general Gaussian kernel, does not learn the time translation of the first spike but changes the space values, i.e., one spike disappears before emerging at a translated position. At the same time, TS-LDDMM handles the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

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

40 However, a graph time series transformation by a general diffeomorphism is not always a graph time  
 41 series, see e.g. Figure 1, thus a graph time series is more than a simple curve [21]. Our contributions  
 42 arise from this observation: we specify the class of diffeomorphisms to consider and show how to  
 43 learn them. This change is fruitful in representing transformations of time series graphs as illustrated  
 44 in Figure 2.

45 Our contributions can be summarized as follows:

- 46 • We propose an unsupervised method (TS-LDDMM) to analyze the inter-individual vari-  
 47 ability of shapes in a time series dataset (Section 4). In particular, the method can handle  
 48 multivariate time series *irregularly sampled* and with *variable sizes*.
- 49 • We motivate our extension of LDDMM to time series by introducing a theoretical framework  
 50 with a representation theorem for time series graph (Theorem 1) and kernels related to their  
 51 structure (Lemma 1).
- 52 • We demonstrate the identifiability of the model by estimating the true generating parameter of  
 53 synthetic data, and we highlight the sensitivity of our method concerning its hyperparameters  
 54 (Appendix G.1), also providing guidelines for tuning (Appendix D).
- 55 • We highlight the *interpretability* of TS-LDDMM for studying the inter-individual variability  
 56 in a clinical dataset (Section 5).
- 57 • We illustrate the quantitative interest of such representation on classification tasks on real  
 58 shape-based datasets with regular and irregular sampling (Appendix H-??).

## 59 2 Notations

60 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  
 61  $C^m(I, E)$  the set of  $m$ -times continuously differentiable function defined on an open set  $U$  to a normed  
 62 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  
 63 set of positive integers.

### 64 3 Background on LDDMM

65 In this part, we expose how to learn the diffeomorphisms  $(\phi_j)_{j \in [N]}$  using LDDMM, initially intro-  
 66 duced in [5]. In a nutshell, for any  $j \in [N]$ ,  $\phi_j$  corresponds to a differential flow related to a learnable  
 67 velocity field belonging to a well-chosen Reproducing Kernel Hilbert Space (RKHS).

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

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

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

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

78 where the velocity field is  $v : \tau \in [0, 1] \mapsto v_\tau \in \mathbf{V}$  and  $\mathbf{V}$  is a Hilbert space of continuously  
 79 differentiable function on  $\mathbb{R}^{d'}$ . If  $\|du\|_\infty + \|u\|_\infty \leq \|u\|_\mathbf{V}$  for any  $u \in \mathbf{V}$  and  $v \in L^2([0, 1], \mathbf{V}) =$   
 80  $\{v \in C^0([0, 1], \mathbf{V}) : \int_0^1 \|v_\tau\|_\mathbf{V}^2 d\tau < \infty\}$ , by [20, Theorem 5]  $\phi^v$  exists and belongs to  $\mathcal{D}(\mathbb{R}^{d'})$ , where  
 81 we denote by  $\mathcal{D}(\mathbf{O})$  the set of diffeomorphism defined on an open set  $\mathbf{O}$  to  $\mathbf{O}$ . Therefore, for any  
 82 choice of  $v$ ,  $\phi^v$  defines a valid deformation. This offers a general recipe to construct diffeomorphism  
 83 given a functional space  $\mathbf{V}$ .

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

89 It has been proposed in [38] to interpret  $\mathbf{V}$  as a tangent space relative to the group of diffeomorphisms  
 90  $\mathbf{H} = \{\phi^v : v \in L^2([0, 1], \mathbf{V})\}$ . Following this geometric point of view, geodesics can be constructed  
 91 on  $\mathbf{H}$  by using the following squared norm

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

92 By deriving differential constraints related to the minimum of (2) and using Cauchy-Lipschitz  
 93 conditions, geodesics can be defined only by giving the starting point and the initial velocity  $v_0 \in \mathbf{V}$   
 94 [38], as straight lines in Euclidean space. Denoting by  $w(v_0)$  the geodesic starting from the identity  
 95 with initial velocity  $v_0$ , the exponential map is defined as  $\varphi^{\{v_0\}} \triangleq \phi^v$  and the previous matching  
 96 problem becomes a *geodesic shooting problem*:

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

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

100 **Discrete parametrization of diffeomorphism.** In this part,  $\mathbf{V}$  is chosen as an RKHS [6] generated  
 101 by a smooth kernel  $K$  (e.g., Gaussian). We follow [15] and define a discrete parameterization of the  
 102 velocity fields to perform geodesics shooting (3). The initial velocity field  $v_0$  is chosen as a finite  
 103 linear combination of the RKHS basis vector fields,  $\mathbf{n}_0$  control points  $\mathbf{X}_0 = (x_{k,0})_{k \in [\mathbf{n}_0]} \in (\mathbb{R}^{d'})^{\mathbf{n}_0}$   
 104 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  $x \in \mathbb{R}^{d'}$ ,

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

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

105 In our applications, the control points  $(x_{k,0})_{k \in [n_0]}$  can be understood as the discretized graph  
 106  $(t_k, \mathbf{s}_0(t_k))_{k \in [n_0]}$  of a starting time series  $\mathbf{s}_0$ . With this parametrization of  $v_0$ , (author?) [38] show  
 107 that the velocity field  $v$  of the solution of (3) keeps the same structure along time, such that for any  
 108  $x \in \mathbb{R}^{d'}$  and  $\tau \in [0, 1]$ ,

$$109 \quad v_\tau(x) = \sum_{k=1}^{n_0} K(x, x_k(\tau)) \alpha_k(\tau) ,$$

$$\begin{cases} \frac{dx_k(\tau)}{d\tau} = v_\tau(x_k(\tau)) , & \frac{d\alpha_k(\tau)}{d\tau} = - \sum_{l=1}^{n_0} d_{x_k(\tau)} K(x_k(\tau), x_l(\tau)) \alpha_l(\tau)^\top \alpha_k(\tau) \\ \alpha_k(0) = \alpha_{k,0}, & x_k(0) = x_{k,0}, k \in [n_0] \end{cases} \quad (5)$$

110 These equations are derived from the hamiltonian  $H : (\alpha_k, x_k)_{k \in [n_0]} \mapsto \sum_{k,l=1}^{n_0} \alpha_k^\top K(x_k, x_l) \alpha_l$ ,  
 111 such that the velocity norm is preserved  $\|v_\tau\|_V = \|v_0\|_V$  for any  $\tau \in [0, 1]$ . By (5), the velocity  
 112 field related to a geodesic  $v^*$  is fully parametrized by its initial control points and momentum  
 113  $(x_{k,0}, \alpha_{k,0})_{k \in [n_0]}$ . Thus, given a set of targets  $\mathbf{y} = (y_i)_{i \in [T_2]}$  in  $\mathbb{R}^{d'}$ , a set of starting points  $\mathbf{x} =$   
 114  $(x_{i,0})_{i \in [T_1]}$  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  
 115 integration scheme of ODE and a penalty factor  $\lambda > 0$ , the basic geodesic shooting step minimizes  
 116 the following function using a gradient descent method:

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

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

119 **Relation to Continuous Normalizing Flows.** One particular popular choice to address the problem  
 120 of learning a diffeomorphism or a velocity field is Normalizing Flows [45, 30] (NF) or their continuous  
 121 counterpart [11, 22, 46] (CNF). However, we do not rely on this class of learning algorithms for  
 122 several reasons. Indeed, existing and simple normalizing flows are not suitable for the type of data  
 123 that we are interested in this paper [17, 14]. In addition, they are primarily designed to have tractable  
 124 Jacobian functions, while we do not require such property in our applications. Finally, the use of  
 125 a differential flow solution of an ODE (1) trick is also at the basis of CNF, which then consists of  
 126 learning a velocity field to address in fitting the data through a loss aiming to address the problem at  
 127 hand. Nevertheless, the main difference between CNF and LDDMM lies in the parametrization of the  
 128 velocity field. LDDMM uses kernels to derive closed form formula and enhance interpretability while  
 129 NF and CNF take advantage of deep neural networks to scale with large dataset in high dimensions.

## 130 4 Methodology

131 We consider in this paper observations which consist in a population of  $N$  multivariate time series, for  
 132 any  $j \in [N]$ ,  $s^j \in C^1(I_j, \mathbb{R}^d)$ . However, we can only access a  $n_j$ -samples  $\tilde{s}^j = (\tilde{s}_i^j = s^j(t_i^j))_{i \in [n_j]}$   
 133 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**  
 134 **necessarily the same across individuals** and the timestamps can be **irregularly sampled**. We assume  
 135 the time series population is globally homogeneous regarding their "shapes" even if inter-individual  
 136 variability exists. Intuitively speaking, the "shape" of a time series  $s : I \rightarrow \mathbb{R}^d$  is encoded in its graphs  
 137  $G(s)$  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  
 138 time axis is crucial. As a motivating use-case,  $s^j$  can be the time series of a heartbeat extracted from  
 139 an individual's electrocardiogram (ECG), see Figure 2. The homogeneity in a resulting dataset comes  
 140 from the fact that humans have similar shapes of heartbeat [57, 35].

141 **The deformation problem.** In this paper, we aim to study the inter-individual variability in the  
 142 dataset by finding a relevant representation of each time series. Inspired from the framework of shape  
 143 analysis [54], addressing similar problems in morphology, we suggest to represent each time series'  
 144 graph  $G(s^j)$  as the transformation of a reference graph  $G(\mathbf{s}_0)$ , related to a time series  $\mathbf{s}_0 : I \rightarrow \mathbb{R}^d$ , by  
 145 a diffeomorphism  $\phi_j$  on  $\mathbb{R}^{d+1}$ , for any  $j \in [N]$ ,

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

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

149 **Optimization related to (7).** Defining the *discretized graphs* of the time series  $(s^j)_{j \in [N]}$  and a  
 150 discretization of the reference graph  $G(s_0)$  as, for any  $j \in [N]$ ,

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

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

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

152 which is carried out by gradient descent on the control points  $\tilde{G}_0$  and the momentums  $\alpha_j = (\alpha_k^j)_{k \in [n_0]}$   
 153 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.  
 154 The optimization hyperparameter details are given in Appendix E.1. The result of the minimization  
 155  $\tilde{G}_0$  is then considered as the  $n_0$ -samples of a common time series  $s_0$  and the momentums  $\alpha_j$  encoding  
 156  $\phi_j$  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  
 157 analyzed with any statistical or machine learning tools such as Principal Components Analysis (PCA),  
 158 Latent Discriminant Analysis (LDA), longitudinal data analysis and so on.

159 Nevertheless, (8) asks to define a kernel and a loss in order to perform geodesic shooting (6), which  
 160 is the purpose of the following subsection.

#### 161 4.1 Application of LDDMM to time series analysis: TS-LDDMM

162 This section presents our theoretical contribution: we tailor the LDDMM framework to handle time  
 163 series data. The reason is that applying a general diffeomorphism  $\phi$  from  $\mathbb{R}^{d+1}$  to a time series' graph  
 164  $G(s)$  can result in a set  $\phi.G(s)$  that does not correspond to the graph of any time series, as illustrated  
 165 in the Figure 1. Thus, time series graphs have more structure than a simple 1D curve [21] and deserve  
 166 their unique analysis, which will prove fruitful as demonstrated in Section 5.

167 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  
 168 generates deformations preserving the structure of the time series graph. This goal motivates us to  
 169 clarify, in Theorem 1, the specific representation of diffeomorphisms we require before presenting a  
 170 class of kernels that produce deformations with this representation.

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

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

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

182 **Theorem 1.** *Let  $s : J \rightarrow \mathbb{R}^d$  and  $s_0 : I \rightarrow \mathbb{R}^d$  be two continuously differentiable time series*  
 183 *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*  
 184  $\Phi_f \in \mathcal{D}(\mathbb{R}^{d+1})$ ,

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

185 *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*  
 186 *series  $\bar{s}$  such that  $G(\bar{s}) = \Pi_{\bar{\gamma}, \bar{f}}.G(s_0)$*

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

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

188 *As a result,  $\Psi_\gamma$  can be understood as a temporal reparametrization and  $\Phi_f$  encodes the transformation*  
 189 *about the space.*

190 **Choice for the kernel associated with the RKHS  $\mathbb{V}$**  As depicted on Figure 1-2, we can not use  
 191 any kernel  $K$  to apply the previous methodology to learn deformations on time series' graphs. We  
 192 describe and motivate our choice in this paragraph. Denote the one-dimensional Gaussian kernel by  
 193  $K_\sigma^{(a)}(x, y) = \exp(-|x - y|^2/\sigma)$  for any  $(x, y) \in (\mathbb{R}^a)^2$ ,  $a \in \mathbb{N}$  and  $\sigma > 0$ . To solve the geodesic  
 194 shooting problem (6) on  $\mathbb{R}^{d+1}$ , we consider for  $\mathbb{V}$  the RKHS associated with the kernel defined for  
 195 any  $(t, x), (t', x') \in (\mathbb{R}^{d+1})^2$ :

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

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

196 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  
 197 motivated by the representation Theorem 1 and the following result.

198 **Lemma 1.** *If we denote by  $\mathbb{V}$  the RKHS associated with the kernel  $K_G$ , then for any vector field*  
 199  *$v$  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*  
 200  *$\phi^v = \Psi_\gamma \circ \Phi_f$ .*

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

203 **Remark 3.** *With this choice of kernel, the features associated with the time transformation can be*  
 204 *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*  
 205 *time. However, the features related to the space transformation are not only in the space coordinates*  
 206 *since the related kernel  $K_{\text{space}}$  depends on time as well.*

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

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

209 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  
 210 potentially of different sizes  $n_j$  and sampled at different timestamps  $(t_i^j)_{i \in [n_j]}$  for any  $j \in [N]$ . Usual  
 211 metrics, such as the Euclidean distance, are not appealing as they make the underlying assumptions  
 212 of equal size sets and the existence of a pairing between points. Distances between measures on sets  
 213 (taking the empirical distribution), such as Maximum Mean Discrepancy (MMD) [16, 7], alleviate  
 214 those issues; however, MMD only accounts for positional information and lacks information about  
 215 the time evolution between sampled points. A classical data fidelity metric from shape analysis  
 216 corresponding to the distance between *oriented varifolds* associated with curves alleviates this last  
 217 issue [28]. Intuitively, an oriented varifold is a measure that accounts for positional and tangential  
 218 information about the underlying curves at sample points. More details and information about  
 219 *oriented varifolds* can be found in Appendix C.

220 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 kernel<sup>2</sup>  $k :$   
 221  $(\mathbb{R}^{d+1} \times \mathbb{S}^d)^2 \rightarrow \mathbb{R}$  verifying [28, Proposition 2 & 4], for any  $\xi \in \{0, 1\}$  and  $i \in [T_\xi - 1]$ , denoting  
 222 the center and length of the  $i^{\text{th}}$  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  
 223  $\vec{v}_i^\xi = (g_{i+1}^\xi - g_i^\xi)/l_i^\xi$ , the varifold distance between  $G_0$  and  $G_1$  is defined as,

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

$$+ \sum_{i,j=1}^{T_1-1} l_i^1 k((c_i^1, \vec{v}_i^1), (c_j^1, \vec{v}_j^1)) l_j^1$$

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

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

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

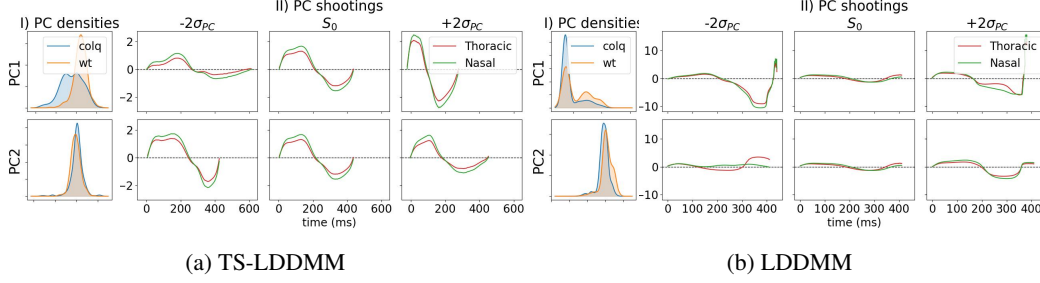


Figure 3: Analysis of the two principal components (PC) related to mice' respiratory cycles before exposure for TS-LDDMM Figure 3a, and LDDMM Figure 3b. In both cases, I) displays PC densities according to mice genotype and II) displays deformations of the reference graph  $S_0$  along each PC.

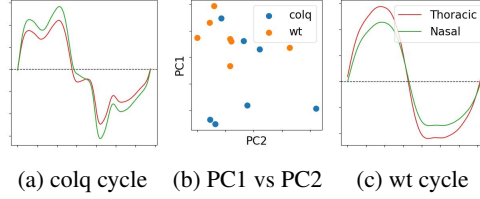


Figure 4: Figure 4a is a **colq** respiratory cycle. Figure 4b displays individual mouse reference respiratory cycle in the TS-LDDMM PC1-PC2 coordinates. Figure 4c is a referent respiratory cycle of a **wt** mouse learned with TS-LDDMM.

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

## 5 Experiments

For conciseness, several experiments are relegated in appendix:

- 1. TS-LDDMM representation identifiability, Appendix G:** On synthetic data, we evaluate the ability of our method to retrieve the parameter  $v_0^*$  that encodes the deformation  $\varphi^{\{v_0^*\}}$  acting on a time series graph  $G$  by solving the geodesic shooting problem (6) between  $G$  and  $\varphi^{\{v_0^*\}}.G$ . **Results** show that TS-LDDMM representations are identifiable or weakly identifiable depending on the velocity field kernel  $K_G$  specification.
- 2. Robustness to irregular sampling, Appendix H:** We compare the robustness of TS-LDDMM representation with 9 URL methods handling irregularly sampled multivariate time series on 15 shape-based datasets (7 univariates & 8 multivariates). We assess methods' classification performances under regular sampling (0% missing rate) and three irregular sampling regimes (30%, 50%, and 70% missing rates), according to the protocol depicted in [29]. **Results** show that our method, TS-LDDMM, outperforms all methods for sampling regimes with missing rates: 0%, 30%, and 50%.
- 3. Classification benchmark on regularly sampled datasets, Appendix I:** We compare performances of a kernel support vector machine (SVC) algorithm based on TS-LDDMM representation with 3 state-of-the-art classification methods from shape analysis on 15 shape-based datasets (7 univariates & 8 multivariates). **Results** show that the TS-LDDMM-based method outperforms other methods (best performances over 13 datasets), making TS-LDDMM representation relevant for time series shape analysis.

### 5.1 Interpretability: analysis of respiratory behavior in mice

This experiment highlights the *interpretability* of TS-LDDMM representation for studying the inter-individual variability in time series biomedical datasets. We consider a multivariate time series dataset

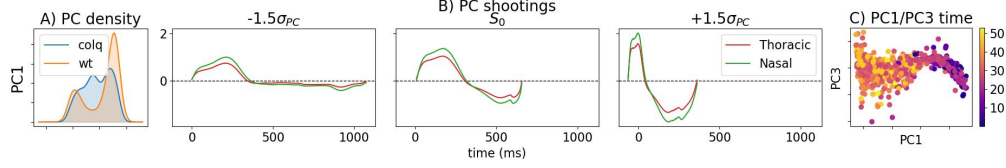


Figure 5: Analysis of the first Principal Component (PC1) related to mice' respiratory cycles before and after exposure for TS-LDDMM. Figure A) displays PC densities according to mice genotype, Figure B) displays deformations of the reference graph  $S_0$  along PC1, and Figure C) displays respiratory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

that accounts for mice's nasal and thoracic airflow evolution when exposed to an irritant molecule altering respiratory functions [39]. The dataset is divided into two groups, one composed of 7 control mice (**wt**) and the other of 7 mice (**colq**) deficient in an enzyme involved in the control of respiration. For each mouse, airflows were recorded for 15 to 20 minutes before exposure to the irritant molecule and then for 35 to 40 minutes. A complete description of the dataset is given in the Appendix F.1.

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

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

**Breathing behaviors' evolution after exposure to the irritant molecule** TS-LDDMM representation features are learned on a dataset that includes respiratory cycles before and after exposure. Figure 5 displays the first principal component PC since it encodes the effect of the irritant molecule as depicted in Figure 5-C) (the exposure occurs at 20 minutes). Figure 5-B) shows that the deformation ( $-1.5 \sigma_{PC}$ ) leads to longer respiratory cycles that include a pause between inspiration and expiration as observed in [19]. Conjointly, Figure 5-A) shows a bimodal distribution for **wt** mice whereas **wt** distributions before exposure were unimodal (Figure 3a). Indeed, the irritant molecule inhibits the action of the deficient enzyme, **wt** mice strongly react to the irritant molecule, whereas **colq** mice better adapt due to their deficiency [19].

## 6 Related Works

Shape analysis focuses on statistical analysis of mathematical objects invariant under some deformations like rotations, dilations, or time parameterization. The main idea is to represent these objects in a complete Riemannian manifold  $(\mathcal{M}, g)$  with a metric  $g$  adapted to the geometry of the problem [38]. Then, any set of points in  $\mathcal{M}$  can be represented as points in the tangent space of their Frechet



mean  $\mathbf{m}_0$  [42, 31] by considering their logarithms. The goal is to find a well-suited Riemannian structure according to the nature of the studied object.

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

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

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

All these state-of-the-art methods previously mentioned [21, 41, 56, 24] are compared to TS-LDDMM in Appendix H and Appendix I.

## 7 Limitations and conclusion

This paper proposes a feature representation method, TS-LDDMM, designed for shape comparison on homogeneous time series datasets. We show on a real dataset its ability to study, with high interpretability, the inter-individual shape variability. As an unsupervised approach, it is user-friendly and enables knowledge transfer for different supervised tasks such as classification.

Although TS-LDDMM is already competitive for classification, its performances can be leveraged on more heterogeneous datasets using a hierarchical clustering extension, which is relegated for future work.

TS-LDDMM employs kernel computations, which require specific libraries (e.g., KeOps [9]) to be efficient and scalable. However, in our experiments, the time complexity of TS-LDDMM is comparable to that of competitors. It is clear that TS-LDDMM needs to be extended to handle very large datasets with high-dimensional time series (such as videos).

Additionally, TS-LDDMM requires tuning several hyperparameters, though this is a common requirement among competitors [21, 41, 56, 24]. In future work, adaptive methods are expected to be developed to provide a more user-friendly interface.

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## A Societal impact

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

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

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

## B Proofs

Denote by  $G(s) \triangleq \{(t, s(t)) : t \in I\}$  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  $\mathbb{V}$  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  $\phi^v = \Psi_\gamma \circ \Phi_f$ .

533 *Proof.* Let  $v$  be a vector field generated by (5) with  $v_0$  satisfying (4). We remark that the first  
534 coordinate of the velocity field  $v_\tau$  denoted by  $v_\tau^{\text{time}}$  only depends on the time variable  $t$  for any  
535  $\tau \in [0, 1]$ . Thus, when computing the first coordinate of the deformation  $\phi^v$ , denoted by  $\gamma$ , we  
536 integrate (1) with  $v_\tau$  replaced by  $v_\tau^{\text{time}}$ , thus  $\gamma$  is independant of the variable  $x$ . Moreover,  $\gamma \in \mathcal{D}(\mathbb{R})$   
537 since a Gaussian kernel induced an Hilbert space  $\mathcal{V}$  satisfying  $|f|_{\mathcal{V}} \leq |f|_{\infty} + |\text{d}f|_{\infty}$  for any  $f \in \mathcal{V}$   
538 by [20, Theorem 9]. For the same reason, we have  $\phi^v \in \mathcal{D}(\mathbb{R}^{d+1})$ , and thus its last coordinates  
539 denoted by  $f$  belongs to  $C^1(\mathbb{R}^{d+1}, \mathbb{R}^d)$ , and by construction  $\phi^v = \Psi_\gamma \circ \Phi_f$ .  $\square$

## 540 C Oriented varifold

541 In this section, we introduce the *oriented varifold* associated with curves. For further readings  
542 on curves and surfaces representation as varifolds, readers can refer to [28, 10]. We associate to  
543  $\gamma \in C^1((a, b), \mathbb{R}^{d+1})$  an *oriented varifold*  $\mu_\gamma$ , i.e. a distribution on the space  $\mathbb{R}^{d+1} \times \mathbb{S}^d$  defined as  
544 follows, for any smooth test function  $\omega : \mathbb{R}^{d+1} \times \mathbb{S}^d \rightarrow \mathbb{R}$ ,

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

545 Denoting by  $W$  the space of smooth test function, we have that  $\mu_\gamma$  belongs to its dual  $W^*$ . Thus,  
546 a distance on  $W^*$  is sufficient to set a distance on oriented varifolds associated to curve and thus  
547 on  $C^1((a, b), \mathbb{R}^{d+1})$  by the identification  $\gamma \rightarrow \mu_\gamma$ . Remark that in (TS-LDDMM),  $\gamma$  should be  
548 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  
549  $s : I \rightarrow \mathbb{R}^d$  the time series. However, in practice, we work with discrete objects. That is why, we  
550 set  $W$  as an RKHS to use its representation theorem. More specifically [28, Proposition 2 & 4]  
551 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  
552 continuously differentiable kernels  $k_{\text{pos}}$  and  $k_{\text{dir}}$ , such that for any  $(x, \vec{u}), (y, \vec{v}) \in (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2$

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

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

555 Given such a kernel  $k : (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2 \rightarrow \mathbb{R}$  verifying [28, Proposition 2 & 4], we have that for any  
556  $(x, v) \in \mathbb{R}^{d+1} \times \mathbb{S}^d$ ,  $\delta_{(x, \vec{v})}$  belongs to  $W^*$  as a distribution and that the dual metric  $\langle \cdot, \cdot \rangle_{W^*}$  satisfies  
557 for any  $(x_1, v_1), (x_2, v_2) \in (\mathbb{R}^{d+1} \times \mathbb{S}^d)^2$ ,

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

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

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

560 we have,

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

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

563 Now, we aim to discretize the oriented varifold  $\mu_G$  related to a time series' graph  $G(s)$  by using a set  
564 of triplets. This is carried out by using a discretized version of  $G(s)$ , i.e.  $\tilde{G} = (g_i = (t_i, s(t_i)))_{i \in [T]} \in$   
565  $(\mathbb{R}^{d+1})^T$ , in the following way: For any  $i \in [T-1]$ , denoting the center and length of the  $i^{\text{th}}$  segment  
566  $[g_i, g_{i+1}]$  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  
567  $\vec{v}_i = (g_{i+1} - g_i)/l_i$ , we define the set of triplets  $X(\tilde{G}) = (l_i, c_i, \vec{v}_i)_{i \in [T-1]}$  and its related oriented  
568 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  $\mu_G$

569 according to [28, Proposition 1]:  $\mu_{X(\tilde{G})}$  converges towards  $\mu_G$  as the size of the discretization mesh  
570  $\sup_{i \in [T-1]} |t_{i+1} - t_i|$  converges to 0.

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

### 573 C.1 Varifold kernels

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

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

577 where  $\sigma_{\text{pos},t}, \sigma_{\text{pos},x}, \sigma_{\text{dir},t}, \sigma_{\text{dir},x} > 0$  are hyperparameters. In practice, we select  $\sigma_{\text{pos},x} \approx \sigma_{\text{dir},x} \approx$   
578 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  
579  $\bar{\sigma}_s$  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  
580 sampling frequency of the time series and  $m \in [5]$  an integer depending on the time change between  
581 the starting and the target time series graph. The more significant the time change, the higher  $m$   
582 should be. The intuition comes from the fact that the width  $\sigma_{\text{pos},t}, \sigma_{\text{dir},t}$  rules the time windows used  
583 to perform the comparison, and  $\sigma_{\text{pos},x}, \sigma_{\text{dir},x}$  affects the space window. The size of the windows  
584 should be selected depending on the variations in the data.

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

586 The parameter  $\sigma_{T,0}$  should be chosen *large* compared the sampling frequency  $f_e$  and compared to  
587 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  
588 time transformation smoother. If  $\sigma_{T,0}$  is too small, for instance,  $\sigma_{T,0} = f_e$ , the effect of the time  
589 deformation is too localized, and there are not enough samples to make it visible.

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

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

## 595 E Experimental settings

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

### 599 E.1 Optimization details of TS-LDDMM & LDDMM

600 We implemented TS-LDDMM in Python with the JAX library<sup>3</sup>.

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

604 **Gradient descent.** The chosen gradient descent method is "adabelief" [60] implemented in the  
605 OPTAX library<sup>4</sup>. The gradient descent has two main parameters: the number of steps (nb\_steps) and  
606 the maximum stepsize value ( $\eta_M$ ). The stepsize has a scheduling scheme:

<sup>3</sup><https://github.com/google/jax>

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

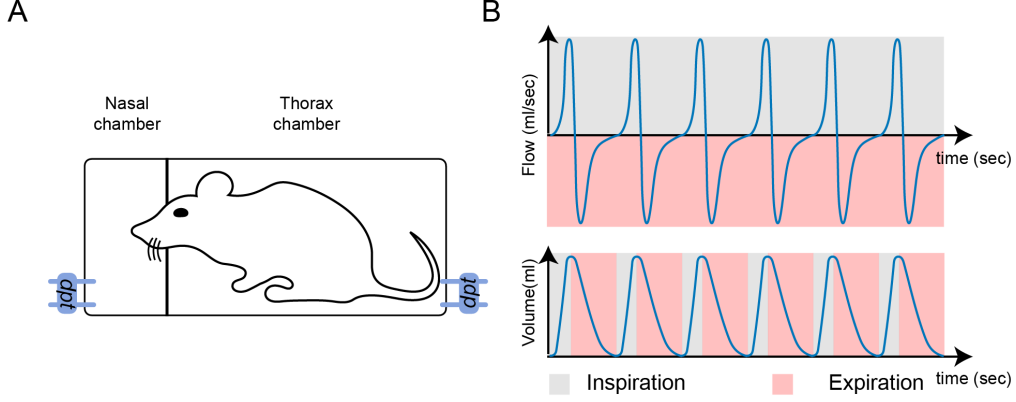


Figure 6: A: Illustration of a double-chamber plethysmograph. The term *dpt* stands for differential pressure transducer which measures the pressure in each compartment, the pressure then being converted to flow. B: Nasal airflow (top) and lung volume (bottom). During inspiration, airflow is positive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

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

By default, we set nb\_steps to 400 and  $\eta_M$  to 0.1.

## F Datasets

### F.1 Mouse respiratory cycle dataset

Ventilation is a simple physiological function that ensures a vital supply of oxygen and the elimination of CO<sub>2</sub>. Acetylcholine (Ach) is a neurotransmitter that plays an important role in muscular activity, notably for breathing. Indeed, muscle contraction information passes from the brain to the muscle through the nervous system. Achs are located in synapses of the nervous system (central and peripheral) and skeletal muscles. They ensure the information transmission from nerve to nerve. However, the transmission cannot end without the hydrolysis of Ach by the enzyme Acetylcholinesterase (AChE), allowing nerves to return to their resting state. Inhibition of (AChE) with, for instance, nerve gas, pesticide, or drug intoxication leads to respiratory arrests.

The dataset comes from the experiment [39], where they studied the consequences of partial deficits in AChE and AChE inhibition on mice respiration. AChE inhibition was induced with an irritant molecule called physostigmine (an AChE inhibitor). Mice nasal airflows were sampled at 2000Hz with a Double Chamber plethysmograph [26], as depicted in Figure 6-A). The flow is expressed in  $ml.s^{-1}$ ; it has a positive value during inspiration and a negative value expiration Figure 6-B). Among the mice population, we selected 7 control mice (**wt**) and 7 ColQ mice (**colq**), which do not have AChE anchoring in muscles and some tissues. As described in [39], mice experiments were as follows:

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

Respiratory cycles were extracted following procedure [19]. We removed respiratory cycles whose duration exceeds 1 second; the average respiratory cycle duration is 300 ms. We randomly sampled



10 respiratory cycles per minute and mouse. It leads to a dataset of 12,732 (time, genotype)-annotated respiratory cycles.

## F.2 Shape-based UCR/UEA time series classification datasets

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

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

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

## G Appendix for experiment: TS-LDDMM representation identifiability

In this experiment, we evaluate the ability of TS-LDDMM to retrieve the parameter  $v_0^*$  that encodes the deformation  $\varphi^{\{v_0^*\}}$  acting on a time series graph  $G$  by solving the geodesic shooting problem (6) between  $G$  and  $\varphi^{\{v_0^*\}}.G$ . Parameter identifiability is an important property for subsequent statistical analysis. Results show that TS-LDDMM representations are identifiable or weakly identifiable depending on the velocity field kernel  $K_G$  specification.

### G.1 Settings

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

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

provided that the hyperparameters and the reference graph are wisely selected, i.e., the parameter  $v_0^*$  generating a deformation  $\varphi^{\{v_0^*\}}$  of a time series graph  $G$  can be estimated from the data  $G, \varphi^{\{v_0^*\}}.G$  by solving the geodesic shooting problem (6).

**The velocity field kernel  $K_G$  is well specified.** First, we show the model identifiability when the kernel  $K_G$  is well specified: the estimated parameter is a good approximation of the generating parameter when the generation and the estimation procedure use the same hyperparameters for

<sup>5</sup><https://timeseriesclassification.com>

<sup>6</sup><https://www.aeon-toolkit.org/en/stable/>

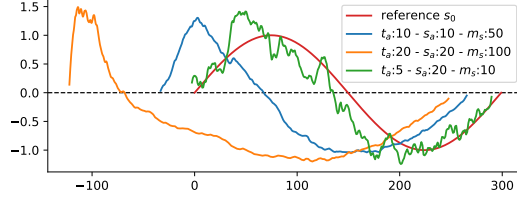


Figure 7: Plots of  $\varphi^{\{v_0(\alpha^*, X)\}} \cdot X$  for different values of  $\alpha^*$  according to its sampling parameter  $t_a, s_a, m_s$ , taking  $X = G(s_0)$  with  $s_0 : k \in [300] \rightarrow \sin(2\pi k/300)$ .

Table 2: Values of  $\mathcal{L}(\varphi^{\{v_0(\alpha^*, X)\}} \cdot X, \varphi^{\{\hat{v}_0\}} \cdot X)$  as  $\alpha^*$  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

the RKHS kernel  $K_G$ . All the hyperparameter values for generation and estimation are given in Appendix G.1.

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  $k \in [n_0]$ ,  $\alpha_k^*$  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  $\alpha^*$  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  $\alpha_k^*$  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  $\alpha^*$  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  $\alpha^*$  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 7: this impacts the Varifold loss which is sensitive to tangents.

**The velocity field kernel  $K_G$  is misspecified.** 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  $\alpha^*$  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 2 that the reconstruction is almost perfect except in the case when  $\sigma_{T,0} = 1$  during estimation, while  $\sigma_{T,0} = 100$  during generation. Compared to  $\sigma_{T,0}$ ,  $\sigma_x$  has nearly no impact on the reconstruction. In Appendix C.1-D, we propose guidelines to drive future hyperparameters tuning and further discussions related to  $\sigma_{T,1}, c_0, c_1$ .

## H Appendix for experiment: Robustness to irregular sampling

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

### H.1 Benchmark methods

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

- RNN-based methods: Baseline recurrent neural networks including RNN [36], LSTM [25], and GRU [12].
- Attention-based methods: Multi-Time Attention Networks (MTAN) [49] and Multi-Integration Attention Module (MIAM) [33]. Both handle multivariate time series irregularly sampled with attention mechanisms.
- Neural ODEs: ODE-LSTM [32] a form of Neural-ODEs used to learn continuous latent representations.
- Neural SDEs: Neural SDE [34] and Neural LNSDE [41] have been proposed to model randomness in time-series using drift and diffusion terms as an extension of Neural-ODEs.
- Shape-Analysis methods: TS-LDDMM (ours) and LDDMM [21]. From shape analysis, both methods learn representations by solving ODEs parametrized with Kernels. While both methods handle multivariate signals irregularly sampled, TS-LDDMM is specifically designed for time series.

### H.2 Model architecture

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

For each method and dataset, the learning rate, the hidden vector dimensions, and the number of layers are optimized to minimize the CrossEntropy loss on a validation set using the Ray<sup>8</sup> Python library. The learning rate varies from  $10^{-4}$  to  $10^{-1}$  using log uniform search, the hidden vector dimension ranges from 16, 32, 64, 128 using grid search, and the number of layers ranges from 1, 2, 3, 4 using grid search. The batch size was selected from 16, 32, 64, 128 according to the size of the dataset. All methods were trained for 100 epochs, and the best method was selected based on the lowest validation loss.

**TS-LDDMM and LDDMM** Representations learned with TS-LDDMM or LDDMM are fed to a Support Vector Classifier (SVC) from `scikit-learn`<sup>9</sup>. All SVC’s hyperparameters are set to default except the regularization term C, which is set through grid search on a validation set with the macro f1-score<sup>10</sup>.

To learn TS-LDDMM (resp. LDDMM) representations, the velocity field kernel  $K_G$  is set to  $(c_0, c_1, \sigma_{T,0}, \sigma_{T,1}, \sigma_x) = (1, 0.1, 0.33\bar{l}, 1, n_d)$ , (resp.  $(\sigma_T, \sigma_x) = (0.33\bar{l}, n_d)$ ) where  $\bar{l}$  is the average time series length and  $n_d$  the number of dimensions. For both methods and all datasets, the varifold loss kernels  $(k_{pos}, k_{dir})$  are identical and set to  $(\sigma_{pos,t}, \sigma_{pos,t}, \sigma_{dir,t}, \sigma_{dir,x}) = (2, n_d, 2, n_d)$ . For TS-LDDMM (resp. LDDMM), the optimizer is set with 400 epochs (resp. 400) and a maximum learning rate  $\eta_M = 0.1$  (resp.  $\eta_M = 0.01$ ). In all cases, the initial reference graph is selected in the dataset as a time series with the median length.

<sup>7</sup><https://github.com/yongkyung-oh/Stable-Neural-SDEs>

<sup>8</sup><https://github.com/ray-project/ray>

<sup>9</sup><https://scikit-learn.org/stable/>

<sup>10</sup>[https://scikit-learn.org/stable/modules/generated/sklearn.metrics.f1\\_score.html](https://scikit-learn.org/stable/modules/generated/sklearn.metrics.f1_score.html)

### H.3 Protocol

In this experiment, we investigate the robustness to missing samples and the classification performance of TS-LDDMM compared to Neural ODEs on 15 datasets described in Appendix F.2. For fairness between methods of different architectures, the evaluation protocol on each dataset and method is as follows:

1. Spilt the dataset in train 75%, validation 15%, and test 15%.
2. Tune hyperparameters with train and validation sets and a missing rate of 0%.
3. For each missing rate in [0%,30%,50%,70%]
  - Remove samples in time series in the train and test sets according to the missing rate and the drop procedure described in [29].
  - Train the model on the train set
  - Evaluate the macro f1-score on the test set

### H.4 Results

In this experiment, we investigate the robustness to missing samples and the classification performance of TS-LDDMM representations. We compare TS-LDDMM with LDDMM and 8 neural ODEs networks. Performances are evaluated in terms of average macro f1-score and rank on four different regimes of missing rate 0%,30%,50%, and 70%. Results are aggregated in Table 3.

On three out of four regimes (0%,30%, and 50%) TS-LDDMM classifier is the best performer in terms of f1-score and rank. For missing rates of 0% and 30%, the score increases by 10% compared to the second-best performer, LDDMM. However, LDDMM is not the second-best performer in rank (Neural LNSDE), showing its sensitivity to parameterization, unlike TS-LDDMM, which remains consistent. Performances of Neural LNSDE remain constant with the increase of the missing rate as observed in [41], and it becomes the best performer for missing rate 70%. The decrease in TS-LDDMM performances with the increasing missing rate is due to the varifold loss, which poorly approximates the time series shape. Other losses might be more relevant for high missing rates.

Overall, TS-LDDMM is a relevant and consistent shape-based representation for irregularly sampled multivariate time series for missing rates up to 50% .

Table 3: Comparison of average macro f1-score and rank as the sample dropping rate increases. **First & second best performers.** TS-LDDMM is the best performer on three out of four regimes.

Methods	Regular		30 % dropped		50 % dropped		70 % dropped	
	F1-score	Rank	F1-score	Rank	F1-score	Rank	F1-score	Rank
RNN (1999)	$0.64 \pm 0.21$	6.2	$0.53 \pm 0.23$	6.6	$0.48 \pm 0.21$	7.2	$0.44 \pm 0.21$	6.07
LSTM (1997)	$0.61 \pm 0.29$	6.0	$0.57 \pm 0.29$	6.27	$0.53 \pm 0.25$	6.07	$0.51 \pm 0.29$	5.27
GRU (2014)	$0.71 \pm 0.26$	4.2	$0.68 \pm 0.28$	4.27	$0.66 \pm 0.28$	3.73	$0.59 \pm 0.28$	<u>3.67</u>
MTAN (2021)	$0.59 \pm 0.28$	7.13	$0.58 \pm 0.28$	5.8	$0.54 \pm 0.29$	5.33	$0.51 \pm 0.28$	5.0
MIAM (2022)	$0.48 \pm 0.35$	6.93	$0.42 \pm 0.33$	8.27	$0.47 \pm 0.31$	6.93	$0.35 \pm 0.31$	7.6
ODE-LSTM (2020)	$0.63 \pm 0.24$	6.0	$0.57 \pm 0.25$	6.53	$0.51 \pm 0.24$	7.27	$0.45 \pm 0.23$	6.73
Neural SDE (2019)	$0.48 \pm 0.28$	7.67	$0.47 \pm 0.26$	7.47	$0.45 \pm 0.27$	7.13	$0.45 \pm 0.25$	6.0
Neural LNSDE (2024)	$0.7 \pm 0.27$	<u>3.87</u>	$0.68 \pm 0.29$	<u>4.0</u>	$0.67 \pm 0.25$	<u>3.53</u>	<b><math>0.66 \pm 0.23</math></b>	<b>2.47</b>
LDDMM (2008)	<u><math>0.72 \pm 0.2</math></u>	4.53	<u><math>0.7 \pm 0.21</math></u>	4.2	$0.57 \pm 0.25$	5.0	$0.4 \pm 0.25$	7.13
TS-LDDMM (ours)	<b><math>0.83 \pm 0.18</math></b>	<b>2.93</b>	<b><math>0.8 \pm 0.18</math></b>	<b>2.07</b>	<b><math>0.7 \pm 0.26</math></b>	<b>3.33</b>	$0.51 \pm 0.27$	5.67

## I Appendix for experiment: Classification benchmark on regularly sampled datasets

In this section, we compare the classification performances of TS-LDDMM with other methods from shape analysis on 15 shape-based datasets of time series regularly sampled. TS-LDDMM outperforms other methods on 12 out of 15, highlighting its relevance for shape analysis when dealing with time series.

## I.1 Benchmark methods

- SRV-based method: we include TCLR [24] a logistic regression on the tangent space of the Frechet mean with Square Root Velocity (SRV representation). We also include Shape-FPCA [56] that encodes both the time series and its time parameterization.
- LDDMM-Based : TS-LDDMM (ours) and LDDMM [21]. Both methods learn representations by solving ODEs parametrized with Kernels. While both methods handle multivariate signals, TS-LDDMM is specifically designed for time series.

## I.2 Model settings

**TCLR & Shape-FPCA** Shape-FPCA is available in the Python library FDASRSF<sup>11</sup>. Once the shape-FPCA representations are learned, they are fed to an SVC from `scikit-learn`. FDASRSF provides SRV representation methods that we combined with a logistic regression from `scikit-learn` to implement TCLR. For both methods, the number of steps to learn the Frechet mean is set to 50, and the regularization hyperparameter C is set through grid search on a validation set with the macro f1-score. Other parameters are set to default.

**TS-LDDMM & LDDMM** Representations learned with TS-LDDMM or LDDMM are fed to an SVC from `scikit-learn`. All SVC’s hyperparameters are set to default except the regularization term C, which is set through grid search on a validation set with the macro f1-score.

To learn TS-LDDMM (resp. LDDMM) representations, the velocity field kernel  $K_G$  is set to  $(c_0, c_1, \sigma_{T,0}, \sigma_{T,1}, \sigma_x) = (1, 0.1, 0.33\bar{l}, 1, n_d)$ , (resp.  $(\sigma_T, \sigma_x) = (0.33\bar{l}, n_d)$ ) where  $\bar{l}$  is the average time series length and  $n_d$  the number of dimensions. For both methods and all datasets, the varifold loss kernels  $(k_{pos}, k_{dir})$  are identical and set to  $(\sigma_{pos,t}, \sigma_{pos,t}, \sigma_{dir,t}, \sigma_{dir,x}) = (2, n_d, 2, n_d)$ . For TS-LDDMM (resp. LDDMM), the optimizer is set with 400 epochs (resp. 400) and a maximum learning rate  $\eta_M = 0.1$  (resp.  $\eta_M = 0.01$ ). In all cases, the initial reference graph is selected in the dataset as a time series with the median length.

**Protocol** For each dataset and method, the evaluation protocol is a simple train, validation test with hyperparameter tuning:

1. Split The dataset in train 75%, validation 15%, and test 15%.
2. Training and hyperparameters tuning with train and validation sets
3. Evaluate the macro f1-score on the test set

## I.3 Results

In this experiment, we investigate the classification performances of several methods from shape analysis on 15 shape-based time series datasets (7 univariate and 8 multivariate). The performances are evaluated in terms of macro f1-score. Results are aggregated in Table 4.

The TS-LDDMM-based classifier outperforms other methods on 12 out of 15 datasets. TCLR is the second-best performer on univariate datasets; however, its current implementation with FDASRSF does not extend to the multivariate case, which limits usage. LDDMM performances are lower than TCLR, and Shape-FPCA is the worst performer.

Overall, TS-LDDMM representations are well suited for shape-based time series classification, and its extension to multivariate irregularly sampled time series makes it a relevant option for time series shape analysis.

## J Appendix for experiment: Analysis of respiratory behavior in mice

### J.1 Settings

This experiment involves TS-LDDMM and LDDMM [21] methods. Both methods are run twice, first on respiratory cycles before exposure to the irritant molecule to capture mice breathing behavior

<sup>11</sup><https://fdasrsf-python.readthedocs.io/en/latest/>

Table 4: F1-score comparison between methods from shape analysis on 15 datasets. **First** and second best performers.

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

at rest and on all respiratory cycles to capture the influence of the irritant molecule. Exposure to the irritant molecule leads to significant shape deformation in the respiratory cycles, and the terms must be added to the varifold loss to capture deformations at a large time scale.

#### TS-LDDMM parameters.

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

**LDDMM parameters.** Note that varifold losses are unchanged between TS-LDDMM and LD-DMM. Compared to TS-LDDMM, the convergence of LDDMM is more sensitive to the maximum stepsize  $\eta_m$ , which must remain small for LDDMM to guarantee the convergence.

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

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