A Second-Order Model for Time-Dependent Data Interpolation: Splines on Shape Spaces

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Abstract. This article presents a mathematical framework recently developed to perform deterministic interpolation on time-indexed sequences of 2D or 3D shapes. Most of current models in use can be compared to linear interpolation for one dimensional data. We develop a spline interpolation method which is the equivalent of splines interpolation in the Euclidean space, but in the widely developed framework of large deformations by diffeomorphisms. We open some preliminary statistical perspectives for the study of cross-evolution data.

1 Introduction

Mathematical and statistical modeling of shapes has undergone significant development over the past twenty years, driven by a wide range of applications in medical imaging. Initially the focus was on the comparison between two shapes also referred to as registration. Among others, registration and comparison tools derived from a Riemannian point of view on shapes spaces and diffeomorphic transport have been actively developed during the past few years. This framework was used to represent shapes and study the statistical variation of static shapes within a population. An emerging question of interest is now to study time dependent data of shapes (images, landmarks, surfaces or tensors). The basic dataset is then a sequence of shapes indexed by time. For example, a practical application would be the analysis of follow-up studies in brain imaging.

Several attempts models for the variability of longitudinal data have been proposed recently: a parametric model of growth is proposed in [7, 8], which aims to describe the biological evolution as an iteration of random elementary diffeomorphisms, so called GRID. Focusing on image data, statistical estimation of the parameters are performed with the GRID model in [13, 15]. Other attempts are often based on using an initial registration tool (such as geodesics on a group of diffeomorphisms, see [17] for a large overview) to interpolate the time dependent data with piecewise geodesics [5,11]. In [5], the model is further developed with the introduction of time realignments to allow the study of an
ensemble of longitudinal data and the computation of an averaged space-time evolution.

From the modeling point of view a typical growth evolution might be usually smooth in time. However, the piecewise geodesic models underlying current analysis of time dependent shape data can not prevent a loss of regularity at the observation points. Moreover, from a more classical statistical point of view, piecewise linear regression does not provide the best interpolation and extrapolation results. The question of time interpolation was addressed in [3] with the use of a kernel on the time variable but still with underlying piecewise geodesics on the data. Random evolutions of shapes have been treated for instance in [4,10], but here again the model is of first order in the sense that the evolution is not smooth in time. Under this assumption of smooth evolutions of the shape, a second-order model is a proper answer way to circumvent this flaw of the standard piecewise geodesic interpolation. We present the strategy adopted in [16] to perform the second-order interpolation of splines on shape spaces. Note that in this paper [16], we further discussed the link with stochastic modeling and we proposed a Hamiltonian formulation of the method on homogeneous spaces.

After an introduction to the context of splines and the large deformation by diffeomorphisms framework in Section 2, we present the interpolation method in finite dimension in Section 3. We illustrate some properties of the model with several simulations in different situations of interest in Section 4. Compared to [16], we discuss further the stochastic and statistical counterpart of the spline model in Section 5 and Section 6.

2 Preliminary tools

2.1 A variational approach to cubic splines

Since the introduction of splines by I.Schoenberg in [14], this tool is now widespread in applied mathematics and statistics. Interestingly, a variational approach to splines first appeared in [9]. This formulation will be easily generalized to the large deformations by diffeomorphisms framework. We present the following theorem due to Holladay in [9] as a definition of classical splines:

**Theorem 1 (Holladay, 1957)** Let $I = [a, b] \subset \mathbb{R}$ be an interval and $H^2(I)$ be the classical Sobolev space of order 2. Let also $a \leq t_1 \leq \ldots \leq t_n \leq b$ with $n \geq 2$ be $n$ interpolating times and $\{z_1, \ldots, z_n\} \subset \mathbb{R}$ be $n$ real numbers.

There exists a unique $s_0 \in H^2(I)$ minimizing $\int_a^b [s''(t)]^2 \, dt$ among the interpolating curves $s$, i.e. $s \in H^2(I)$ such that $s(t_i) = z_i$ for $i \in [1, n]$.

Furthermore, $s_0 \in C^2(I)$, $s_0$ is a cubic polynomial function on $[t_i, t_{i+1}]$ for $i \in [1, n-1]$ and $s_0$ is an affine polynomial function on $[a, t_1]$ and $[t_n, b]$.

Many generalizations of splines have been proposed since its introduction, for instance higher-order splines are well-known. However, a recent generalization that arises from robotic applications is the extension to the Riemannian setting by Noakes in [12]. In this context, the authors in [12] replace the acceleration
of the Euclidean case $[s^n]^2$ with $\nabla_s s^2_g$ where $g$ is the metric of the Riemannian manifold and $\nabla$ the corresponding Levi-Civita connection.

Interestingly, the approach in [16] was not derived as an application of this procedure although it turns out to be completely equivalent to the Riemannian splines of [2, 12] but in the context of large deformations by diffeomorphisms following a Hamiltonian approach.

### 2.2 Geodesic equations on the landmark space

The problem of landmark matching via diffeomorphic transport is now quite well understood. The basic idea is to build a continuous path of minimal length $\phi_t$ starting from $\phi_0 = 1d_{\mathbb{R}^d}$ in a group $G_V$ of diffeomorphisms, between an initial configuration $x = (x_i)_{1 \leq i \leq n}$ of $n$ landmarks in $\mathbb{R}^d$ and a target configuration $y = (y_i)_{1 \leq i \leq n}$. Thus, if $x_{i,t} = \phi_t(x_i)$ and $x_t = (x_{i,t})_{1 \leq i \leq n}$, $x_t$ is a path from $x$ to $y$ in the space of landmark configurations induced by a geodesic in a Riemannian space of diffeomorphisms. The group $G_V$ is defined through the flow of time dependent velocity fields $(t,x) \to \nu_t(x)$ on $\mathbb{R}^d$

$$\frac{\partial \Phi}{\partial t} = \nu_t \circ \Phi$$

where $V$ is a Hilbert space of velocity fields and $\nu \in L^2([0,1], V)$ is an element of the space of time dependent velocity fields with finite $L^2$ norm. Obviously, the existence of a flow $t \to \Phi_t^\nu$ for $\nu \in L^2([0,1], V)$ solution of (1) depends on some regularity assumptions of the instantaneous velocity fields $\nu_t$, namely the control of the first order derivatives of $\nu_t$. Assuming this, the group $G_V$ is defined as $G_V = \{ \Phi_t^\nu \mid \nu \in L^2([0,1], V) \}$ and the diffeomorphic matching problem for landmarks is formulated through the following variational problem

$$\begin{cases}
\min \int_0^1 |\nu_t|^2_V dt, & \nu \in L^2([0,1], V) \\
\text{with} & \\
\Phi_t^\nu(x_i) = y_i, & 1 \leq i \leq n.
\end{cases} \tag{2}$$

The problem (2) is well posed as soon as $V$ is continuously embedded in $C^1_0([0,1], \mathbb{R}^d)$ the space of $C^1$ velocities vanishing at $\infty$ (such a $V$ is called an admissible space). Namely, we assume the existence of a constant $C$ such that for any $\nu \in V$, the following inequality is verified

$$|\nu|_{1,\infty} \leq C|\nu|_V. \tag{3}$$

Such an admissible space is a Reproducible Kernel Hilbert Space (RKHS) and is equipped with a kernel $K_V(z, z')$ playing a key role in defining the structure of the solution of the geodesic emerging from (2). Since the reader may not be familiar with RKHS, let us say in a nutshell that for any $z, z' \in \mathbb{R}^d$ the kernel $K_V(z, z')$ is a $d \times d$ matrix in $\mathcal{M}_d(\mathbb{R})$, that $z \to K_V(z, z')\alpha' \in V$ for any $z', \alpha' \in \mathbb{R}^d$, that $\langle K_V(., z')\alpha', K_V(., z'')\alpha'' \rangle_V = \alpha'^T K_V(z', z'')\alpha''$ (the so called reproducing property) and that $\langle v, K_V(., z')\alpha' \rangle_V = \langle v(z'), \alpha' \rangle_V$ for any $v \in V$. 

The main fact is that given $K_V$, the space $V$ is completely defined and one may start from the choice of the kernel $K_V$ itself to define the space $V$. A large number of kernels have been proposed most commonly the Gaussian kernel

$$K_V(z, z') = \exp(-\frac{|z - z'|^2}{\lambda^2})\text{Id}_{\mathbb{R}^d}.$$ (4)

Even more importantly, the kernel appears explicitly in geodesics emerging from (2) as described by the following Theorem. To ensure the existence of a solution in this theorem, we need to assume that the kernel is positive definite:

$$\sum_{i=1}^l K_V(x_i, \ldots, x_i) \alpha_i^2_V = 0 \Rightarrow \forall \ i \alpha_i = 0.$$ (5)

**Theorem 2 (cf [6])** The solution $v \in L^2([0, 1], V)$ exists and satisfies

$$v_t(z) = \sum_{i=1}^n K_V(z, x_{i,t})p_{i,t}$$ (6)

where $t \rightarrow (x_{t}, p_{t})$ is solution of

$$\begin{cases}
\dot{x}_t = \frac{\partial H_0}{\partial p}(x, p_t) \\
\dot{p}_t = -\frac{\partial H_0}{\partial x}(x, p_t) + u_t
\end{cases}$$ (7)

with $H_0(p, x) = \frac{1}{2} \sum_{i,j} p_i^T K_V(x_i, x_j) p_j$ and $x_0 = x$.

It is rather standard to prove that this approach endows the landmark space (set of groups of distinct points) with a Riemannian metric which is induced from the one on the group of diffeomorphisms. More generally once a positive definite kernel is given, it gives rise to a Riemannian metric on the space of landmarks, namely $[K_V(x_i, x_j)]_{i,j \in [1, n]}$. Therefore, the Riemannian spline approach could be directly applied in this framework to interpolate smoothly time-dependent diffeomorphic evolution. However, we originally introduced our second-order model following a physical modeling approach by adding a forcing term on the evolution (formula (7)) of the momentum $p$ and then minimizing its norm. We present in the next section our second-order interpolation method.

### 3 The shape spline model

We introduce a (time-dependent) control variable $u$ in the evolution of the momentum as follows:

$$\begin{cases}
\dot{x}_t = \frac{\partial H_0}{\partial p}(p_t, x_t) \\
\dot{p}_t = -\frac{\partial H_0}{\partial x}(p_t, x_t) + u_t
\end{cases}$$ (8)
Assume that we are given $M$ samples $(x_t^D)_{k \in [1,M]}$ (with $0 \leq t_1 \leq \ldots \leq t_M \leq 1$) of sparse observations of a trajectory $x_t^D$ maybe subject to noise. The interpolation method consists in the minimisation of the cost functional:

$$\inf_u J(u) = \left\{ \frac{1}{2} \int_0^1 |u_t|^2_X \, dt + \gamma \sum_{k=1}^M |x_{t_k}^D - x_{t_k}|^2 \right\}$$

subject to $(x, p)$ solution of the ODE (8)

Here, $|.|_X$ is a norm that may differ from the metric given by the kernel on the cotangent space. As discussed in [16], the choice of the norm can be related to the structure of the treated data and especially to the noise model on the data. Interestingly, if one chooses the metric given by the kernel, it is proven in [16] that the cost on $u$ and the one in the Riemannian splines case coincide. Hence, our shape spline model is a little more general than the Riemannian splines since we are free to choose an other metric than the natural one.

Remark that the formulation differs from the exact interpolation problem in Thm. 1 since we aim at taking into account the effect of the noise on the observation data and also to enable a generalization to a non-transitive action of the group in infinite dimensions, namely the case of images.

4 Simulations

In all the following simulations, the norm $|.|_X$ will be chosen as the $L^2$ norm. The study of different norms will be addressed elsewhere.

4.1 Comparison with piecewise geodesic interpolation

The first compelling simulation is the comparison between a piecewise-geodesic interpolation and the shape spline interpolation in Fig. 4.1. The synthetic data simulated are 40 points on the unit circle (time 0) which is deformed via different analytic mappings at several interpolation times 1, 1.3, 2 and 2.5. Note that the landmarks are indexed and we did not perform a measure matching.

In Fig. 4.1, we represent a view of the time evolution $(y-$axis) of the initial circle of points. On the left, we remark the sharp edges at the interpolation time-points characteristic of the piecewise geodesic interpolation model. On the right, a spline interpolation is shown in which the initial momentum is null. The color represents the norm of the control variable. Note that if we optimize also on the initial momentum, we obtain the same type of shape.

A more quantitative simulation is given in [16], where we compare the $L^2$ error of the each interpolation when increasing the number of interpolation times. On that particular example, the convergence rates seem quite similar to the Euclidean case.
4.2 Robustness to noise

The robustness to noise is a rather important subject from a practical point of view. Indeed, the noise basically degrades the spatial resolution of the measurements so that the evolution through time of a particular point of the evolving curve may be a sharply broken line. The standard spline approach can be quite efficient in filtering this noise if the time sampling frequency is high enough. This is hardly the case in many important situations. However, neighboring points behave coherently through time and offer an interesting source of spatial redundancy. Much of the large deformation shape space theory involves the integration of spatial redundancy in the comparison between shapes. The shape spline setting, considering shapes as a whole and not as a bag of independent points, keeps this important aspect but adds a time component and considers the problem in the full space-time setting. This robustness to noise is illustrated in Figure 2 where an i.i.d. Gaussian noise with standard deviation $\sigma = 0.1$ is added to each measurement point. Shape splines are computed with two different scale parameters, $\lambda = 0.001$ on the left, $\lambda = 0.6$ on the right.

Fig. 1. Linear interpolation versus shape spline interpolation

Fig. 2. Robustness to noise. An i.i.d. Gaussian noise with standard deviation $\sigma = 0.1$ is added to each measurement point. Shape splines are computed with two different scale parameters, $\lambda = 0.001$ on the left, $\lambda = 0.6$ on the right.
added and a series of shape splines are computed under increasing values of the spatial regularity scale parameter $\lambda$ as introduced in (4). For low values of this parameters (with respect to the overall scale of the shapes) the reconstructed evolution is clearly far from any reasonable solution since the spatial redundancy is hardly taken into account. Increasing the value of $\lambda$ to values in accordance to the scale of the object produces a much better reconstruction of the actual shapes at any observation time but also keeps existing time regularity.

### 4.3 Extrapolation and other simulations

In addition to the norm of the control variable, we also show in Fig. 3 the orthogonal component of the control variable with its algebraic sign. This quantity gives more information than simply the norm of the control: especially, it gives an information on the direction in which the force mainly acts. A contraction is related to a signed control variable in blue and an expansion to a red color. In the geodesic case of curve matching, the momentum is a normal vector field to the curve and the extension to the infinite-dimensional case of curves should keep this property true in the case of splines.

**Fig. 3.** On each row: two different examples of the spline interpolation. In the first column, the norm of the control is represented whereas the signed normal component of the control is represented in the second one. The last column represents the extrapolation.

Another distinguished feature of the usual spline setting which is extended in the shape spline setting is the fact that the extrapolation of the data outside the interval of observation is quite straightforward. Indeed, outside the limits of the observation interval, the value of the control parameter $u$ is set to zero.
and the evolution is naturally extended with a geodesic evolution. Moreover, one can check that $u$ vanishes at the last observation time so that the previous extension is $C^0$ for the control variable $u$ and $C^1$ for the shape variable $x$. In Figure 3, we display a simple example of extrapolation in the last column for two different evolutions. The computed extrapolation appears visually quite natural at both ends. As the case case of indexed landmarks is not the most usual in Computational Anatomy, the last example is an illustration of the case of measure matching on the contour of skulls (2D-profiles of hominids skulls in which only the contour has been selected - source: www.bordalierinstitute.com also used in [5]). We register the evolution Anthropoid monkey - Australopithecus - Homo Habilis - Homo Erectus - Homo Sapiens Sapiens with respect to the time $\{0.0, 1.0, 2.3, 3.3, 4\}$ (respecting the time intervals between the stages of the evolution in millions of year) and we extrapolate on 0.5 m.y. We do not pay to much attention to the interpretation of this last example since our results may be biased by the rigid registration performed before the spline interpolation. However, this new tool can be used in the several cases of application of the large deformation by diffeomorphisms framework.

5 The stochastic shape spline model

The stochastic counterpart of the deterministic shape spline model may be introduced by adding a random perturbation to the calibrated forcing term $u$. This random perturbation may be chosen as a white noise as a first candidate. From the mathematical viewpoint, it is proven in [16] that the standard Hamiltonian system where a noise term is introduced on the momentum variable provides a model to generate random evolutions:

**Theorem 3** Under assumption (3), the solutions of the stochastic differential equation defined by

$$
\begin{align*}
dp_t &= -\partial_x H_0(p_t, x_t)dt + \varepsilon(p_t, x_t)dB_t \\
 dx_t &= \partial_p H_0(p_t, x_t)dt.
\end{align*}
$$

Fig. 4. View in front of the time axis of the spline interpolation of the skulls.

Fig. 5. View along the time axis ($z-$ axis).
are non exploding when $\varepsilon : \mathbb{R}^{nd} \times \mathbb{R}^{nd} \mapsto L(\mathbb{R}^{nd})$ is a Lipschitz and bounded map.

However, what would be more realistic as a first when a set of longitudinal data of the same type is given, would be to calibrate a control variable $u$ and the noise term $\varepsilon$ so that the most simple realistic model would be the following

**Stochastic growth model:**

$$
\begin{align*}
dp_t &= -\partial_x H_0(p_t, x_t)dt + u_t(x_t, p_t)dt + \varepsilon(p_t, x_t)dB_t \\
\partial x_t &= \partial_p H_0(p_t, x_t)dt.
\end{align*}
$$

(11)

Not unexpectedly, the result of Thm. 3 can be extended in this new model under Lipschitz assumption on $u$. We now discuss some synthetic experiments.

**Fig. 6.** The first figure represents a calibrated spline interpolation and the three others are white noise perturbations of the spline interpolation with respectively $\sqrt{n}\varepsilon$ set to $0.25, 0.5$ and $0.75$.

In Fig. 6, we have calibrated the spline interpolation model on 32 landmarks knowing their positions at times $0, 0.4, 1.0, 1.5$. Once the calibrated forcing term $u^c$ is known, we use the model 11 to generate random evolutions. The parameters are set to $u \equiv u^c$ and $\varepsilon = cste$. The noise parameter is renormalized in function of the number of landmarks, i.e. $\sqrt{n}\varepsilon = cste$ to obtain comparable results when increasing the number of landmarks. The color on every figures just indicates the norm of the control variable $u$ and the $z$-axis represents the time. In Fig. 5, we progressively increase the energy of the noise. We remark that the visible perturbations occur after a common evolution at the beginning. As a consequence, it seems reasonable to also introduce a distribution on the initial momentum as mentioned in [16] in order to enhance the model.

### 6 Statistical Modeling

The preceding stochastic process appears as a natural prior on shape evolution and a quite interesting object to be studied from a pure probabilistic point of view. However, in the practical situation of longitudinal data arising in many cases in neuroimaging, it is quite doubtful that the control $u_t$ could simply be
a white noise process. The problem of the statistical estimation of the law of
the couple \((p_0, u)\) where \(p_0\) is the initial momentum and \(u = (u_t)\) from sparse
observations is a challenging and open problem if one looks for a statistically
consistent estimation method in the spirit of [1].

But more simple routes are straightforwardly available through the use of PCA
analysis of a family \((\hat{p}_0^h, \hat{u}^h)\) of pairs obtained on different evolutions starting
from a common template \(x_0\). We present in Fig. 7 a simple illustrative example
on a synthetic learning database where pairs \((\hat{p}_0^h, \hat{u}^h)\) are given as solutions
of the spline variational problem (9) as described previously. The idea is to
generate a new pairs \((p_0, u)\) from the PCA model which are used to feed the ODE
(8). The results are still preliminary but look rather promising. Obviously, the

![Fig. 7. Top row: Four examples of time evolution reconstructions from the ob-
servations at 6 time points (not represented here) in the learning set. Bottom
row: The simulated evolution generated from a PCA model learn from the pairs
\((p_0^k, u^k)\). The comparison between the two rows shows that the synthetised evo-
lutions from the PCA analysis are visually good.](image)

assumption that the observed evolutions as starting from a common template is
quite restrictive. However, the integration of this approach after co-registration
of the different evolution in the spirit of [5] is possible but beyond the scope of
this paper.

7 Conclusion and perspectives

In the finite dimensional case of landmarks, we have presented a second-order
interpolation method that is particularly suitable for sparse (in time) shape data
such that the underlying evolution is smooth in time. This work opens new statis-
tical time regression perspectives and could also benefit from a special treatment
of the time variable as in [5]. The extension to the infinite-dimensional case of
3D-images is another important perspective and should be addressed in future
work. Indeed, the main mathematical obstacles to develop a practical algorithm for splines are essentially the same than for a geodesic shooting algorithm, which is an ongoing work. Last, we have underlined the generic feature of the spline: a higher-order interpolation model. However, there may be other interesting second order models that are worth being studied (at least to reduce the computational cost of the proposed method) and this is also a direct perspective of this work.

References