Geodesic regression and cubic splines on shape spaces

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joint work with Marc Niethammer (geodesic regression) and Alain Trouvé (cubic splines)

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1 Introduction to Large Deformation by Diffeomorphisms Metric Mapping (LDDMM)

2 Interpolation of time sequence of shapes

3 Second order interpolation

4 Shape Splines

5 A generative model for shape evolutions

6 Geodesic regression
Motivation

- Developing geometrical and statistical tools to analyse biomedical shapes,
- Developing the associated numerical algorithms.
Example of problems of interest

*Given two shapes, find a diffeomorphism of $\mathbb{R}^3$ that maps one shape onto the other*
Example of problems of interest

*Given two shapes, find a diffeomorphism of $\mathbb{R}^3$ that maps one shape onto the other*

Different data types and different way of representing them.

**Figure:** Two slices of 3D brain images of the same subject at different ages
Example of problems of interest

Given two shapes, find a diffeomorphism of $\mathbb{R}^3$ that maps one shape onto the other
About Computational Anatomy

Old problems:

1. to find a framework for registration of biological shapes,
2. to develop a statistical analysis in this framework.
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**Action of a transformation group on shapes or images**
Idea pioneered by Grenander and al. (80’s), then developed by M.Miller, A.Trouvé, L.Younes.

*Figure:* deforming the shape of a fish by D’Arcy Thompson, author of *On Growth and Forms* (1917)
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New problems like study of Spatiotemporal evolution of shapes within a diffeomorphic approach
A Riemannian approach to diffeomorphic registration

Several diffeomorphic registration methods are available:

- Free-form deformations B-spline-based diffeomorphisms by D. Rueckert
- Log-demons (X. Pennec et al.)
- Large Deformations by Diffeomorphisms (M. Miller, A. Trouvé, L. Younes)

Only the last one provides a Riemannian framework.
A Riemannian approach to diffeomorphic registration

- $v_t \in V$ a time dependent vector field on $\mathbb{R}^n$.
- $\phi_t \in Diff$, the flow defined by $\partial_t \phi_t = v_t(\phi_t)$.

Action of the group of diffeomorphism $G_0$ (flow at time 1):

$$\Pi : G_0 \times C \to C, \quad \Pi(\phi, X) = \phi.X$$

Right-invariant metric on $G_0$: $d(\phi_{0,1}, \text{Id})^2 = \frac{1}{2} \int_0^1 |v_t|^2 dt$. 
Inexact matching: taking noise into account

Minimizing

\[ J(v) = \frac{1}{2} \int_0^1 |v_t|^2 \, dt + \frac{1}{2\sigma^2} d(\phi_{0,1} \cdot A, B)^2. \]
Inexact matching: taking noise into account

Minimizing

\[ J(v) = \frac{1}{2} \int_0^1 |v_t|^2 \nu \, dt + \frac{1}{2\sigma^2} d(\phi_{0,1} \cdot A, B)^2. \]

In the case of landmarks:

\[ J(\phi) = \frac{1}{2} \int_0^1 |v_t|^2 \nu \, dt + \frac{1}{2\sigma^2} \sum_{i=1}^k \| \phi(x_i) - y_i \|^2, \]
Inexact matching: taking noise into account

Minimizing

\[
J(v) = \frac{1}{2} \int_0^1 |v_t|^2 dt + \frac{1}{2\sigma^2} d(\phi_{0,1} \cdot A, B)^2 .
\]

In the case of landmarks:

\[
J(\phi) = \frac{1}{2} \int_0^1 |v_t|^2 dt + \frac{1}{2\sigma^2} \sum_{i=1}^{k} \|\phi(x_i) - y_i\|^2 ,
\]

In the case of images:

\[
d(\phi_{0,1} \cdot l_0, l_{\text{target}})^2 = \int_U |l_0 \circ \phi_{1,0} - l_{\text{target}}|^2 dx .
\]

Main issues for practical applications:

- choice of the metric (prior),
- choice of the similarity measure.
A Riemannian framework

Proposition

The inexact matching functional

\[ \mathcal{J}(v) = \int_0^1 |v_t|^2 dt + \frac{1}{\sigma^2} d(\phi_{0,1} A, B)^2 \]

leads to geodesics on the orbit of A for the induced Riemannian metric.

Proposition

Left-action \( G \times Q \mapsto Q \) of a group \( G \) endowed with a right-invariant metric induces a Riemannian metric on the orbits of the action and the map \( \Pi_{q_0} : G \ni g \mapsto g \cdot q_0 \in Q \) is a Riemannian submersion.

Consequence: Geodesics downstairs horizontally lift to geodesics upstairs.
A Riemannian framework

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- Statistics on the initial momentum.
Bayesian interpretation

The prior in the functional

\[ \mathcal{J}(v) = \int_0^1 |v_t|^2 dt + \frac{1}{\sigma^2} d(\phi_{0,1}.A, B)^2 \]

suggests a white noise in time for generic evolutions.

**Figure:** Kunita flows

→ Not realistic for evolutions of biological shapes.
Interpolating sparse longitudinal shape data

What we aim to do:

**Within a diffeomorphic framework:**

Let \((S_{t_0}^i, \ldots, S_{t_n}^i)_{i \in [1,n]}\) be a \(n\)-sample of shape sequences indexed by the time \((t_0^i, \ldots, t_n^i) \subset [0,1]\).

Having in mind biological shapes, at least two problems

- To find a deterministic framework to treat each sample. (in which space to study these data?)
- To develop a probabilistic framework to do statistics. (classification into normal and abnormal growth)
A natural attempt

How to interpolate a sequence of data \((S_0, \ldots, S_{t_k})\) (images, surfaces, landmarks ...)

\[ F(v) = \frac{1}{2} \int_0^1 |v_t|^2 V dt + \sum_{j=1}^k |\phi_{t_j}.S_0 - S_{t_j}|^2, \]
A natural attempt

How to interpolate a sequence of data \((S_0, \ldots, S_{t_k})\) (images, surfaces, landmarks ...)

When \(k = 1 \longrightarrow\) standard registration problem of two images: Geodesic on a diffeomorphism group - LDDMM framework (M.Miller, A.Trouvé, L.Younes, F.Beg,...)

\[
\mathcal{F}(v) = \frac{1}{2} \int_0^1 |v_t|^2 dt + |\phi_1.S_0 - S_{t_1}|^2,
\]

\[
\begin{align*}
\phi_0 &= Id \\
\dot{\phi}_t &= v_t(\phi_t).
\end{align*}
\]
A natural attempt

How to interpolate a sequence of data \((S_0, \ldots, S_{t_k})\) (images, surfaces, landmarks \(\ldots\))

When \(k = 1\) \(\rightarrow\) standard registration problem of two images:
Geodesic on a diffeomorphism group - LDDMM framework
(M.Miller, A.Trouvé, L.Younes, F.Beg, \(\ldots\))

\[
\mathcal{F}(v) = \frac{1}{2} \int_0^1 |v_t|^2_V dt + |\phi_1.S_0 - S_{t_1}|^2,
\]

\[
\left\{
\begin{array}{l}
\phi_0 = Id \\
\dot{\phi}_t = v_t(\phi_t).
\end{array}
\right. \tag{1}
\]

Extending it to \(k > 1\),

\[
\mathcal{F}(v) = \frac{1}{2} \int_0^{t_k} |v_t|^2_V dt + \sum_{j=1}^{k} |\phi_{t_j}.S_0 - S_{t_j}|^2,
\]

\(\rightarrow\) piecewise geodesics in the group of diffeomorphisms
Illustration on 3D images

Figure: Slices of 3D volumic images: 33 / 36 / 43 weeks of gestational age of the same subject.
Illustration on 3D images

Video courtesy of Laurent Risser

Figure: Video courtesy of Laurent Risser
Illustration on 3D images

Video courtesy of Laurent Risser

Figure: Representation of the surface - Back of the brain
How to smoothly interpolate longitudinal data

In the Euclidean space:

![Figure: Sparse data from a sinus curve](image-url)
How to smoothly interpolate longitudinal data

In the Euclidean space:

Minimizing the $L^2$ norm of the speed $\rightarrow$ piecewise linear interpolation

Figure: Linear interpolation of the data.
How to smoothly interpolate longitudinal data

In the Euclidean space:

Enforcing the geodesicity constraint

**Figure:** Cubic spline interpolation of the data.
How to smoothly interpolate longitudinal data

In the Euclidean space:

Minimizing the $L^2$ norm of the **acceleration** $\rightarrow$ cubic spline interpolation

**Figure:** Cubic spline interpolation of the data.
What is acceleration in our context?

**First attempt, on the group** in the matching functional:

\[
\mathcal{F}(v) = \frac{1}{2} \int_0^1 |v_t|_V^2 \, dt + |\phi_1 S_0 - S_{t_1}|^2, \quad (2)
\]

Replace the \(L^2\) norm of the speed:

\[
\frac{1}{2} \int_0^1 |v_t|_V^2 \, dt \quad (3)
\]

by the \(L^2\) norm of the acceleration of the vector field:

\[
\frac{1}{2} \int_0^1 \left| \frac{d}{dt} v_t \right|_V^2 \, dt + |\phi_1 S_0 - S_{t_1}|^2, \quad (4)
\]
What is acceleration in our context?

First attempt, on the group in the matching functional:

$$\mathcal{F}(v) = \frac{1}{2} \int_0^1 |v_t|^2_V \, dt + |\phi_1.S_0 - S_t|^2,$$  \hspace{1cm} (2)

Replace the $L^2$ norm of the speed:

$$\frac{1}{2} \int_0^1 |v_t|^2_V \, dt$$  \hspace{1cm} (3)

by the $L^2$ norm of the acceleration of the vector field:

$$\frac{1}{2} \int_0^1 \left| \frac{d}{dt} v_t \right|^2_V \, dt + |\phi_1.S_0 - S_t|^2,$$  \hspace{1cm} (4)

Null cost for this norm $\longrightarrow v_t \equiv v_0$: Incoherent
Correct notion of acceleration

*Acceleration on a Riemannian manifold* $M$: let $c : I \to M$ be a $C^2$ curve. The notion of acceleration is:

$$\frac{D}{dt} \dot{c}(t) = \nabla_{\dot{c}} \dot{c}(= \ddot{c}_k + \sum_{i,j} \dot{c}_i \Gamma_{i,j}^k \dot{c}_j)$$ (5)

with $\nabla$ the Levi-Civita connection.
Correct notion of acceleration

**Acceleration on a Riemannian manifold** $M$: let $c : I \rightarrow M$ be a $C^2$ curve. The notion of acceleration is:

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(5)

with $\nabla$ the Levi-Civita connection.

Riemannian splines: Crouch, Silva-Leite (90’s)

$$\text{On } SO(3) \inf_{c} \int_{0}^{1} \frac{1}{2} |\nabla_{\dot{c}} \dddot{c}|^2_M dt.$$  

(6)

subject to $c(i) = c_i$ and $\dot{c}(i) = v_i$ for $i = 0, 1.$
Correct notion of acceleration

**Acceleration on a Riemannian manifold** $M$: let $c : I \rightarrow M$ be a $C^2$ curve. The notion of acceleration is:

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$$

(5)

with $\nabla$ the Levi-Civita connection.

Elastic Riemannian splines:

$$
\inf c \int_0^1 \frac{1}{2} |\nabla \dot{c} \ddot{c}|_M^2 + \frac{\alpha}{2} |\dot{c}|_M^2 dt.
$$

(6)

subject to $c(i) = c_i$ and $\dot{c}(i) = v_i$ for $i = 0, 1$. 
A modeling question

The Euler-Lagrange equation for Riemannian cubics is

\[ \nabla^3_c \dot{c} + R(\nabla_c \dot{c}, \dot{c}) \dot{c} = 0, \quad (7) \]

where \( R \) is the curvature tensor of the metric.

Remarks

If \( \pi : M \to B \) is a Riemannian submersion then:

geodesics lift to geodesics.

Probably not true for Riemannian cubics . . .
A modeling question

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where \( R \) is the curvature tensor of the metric.

Remarks

*If \( \pi : M \mapsto B \) is a Riemannian submersion then: geodesics lift to geodesics.*

*Probably not true for Riemannian cubics . . .*

In our context of a group action, \( G \times M \mapsto M \):

\[ \Pi_{q_0} : G \ni g \mapsto g \cdot q_0 \in \mathcal{Q} \]

is a Riemannian submersion

Question

*Higher-order on the group (upstairs) or higher-order on the orbit (downstairs)?
The convenient Hamiltonian setting

Hamiltonian equations of geodesics for landmarks:

\[
\text{Geodesics} \quad \begin{cases} 
\dot{p} = -\partial_q H(p, q) \\
\dot{q} = \partial_p H(p, q)
\end{cases} \quad (8)
\]

with \( H(p, q) = H(p_1, \ldots, p_n, q_1, \ldots, q_n) = \frac{1}{2} \sum_{i,j=1}^{n} p_i k(q_i, q_j) p_j \)

and \( k \) is the kernel for spatial correlation.
The convenient Hamiltonian setting

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and \( k \) is the kernel for spatial correlation.

**Lemma**

On a general Riemannian manifold,

\[
\nabla \dot{q} = K(q)(\dot{p} + \partial_q H(p, q))
\]

(9)

where \( \dot{q} = K(q)p \) with \( K(q) \) being the identification given by the metric between \( T_q^*Q \) and \( T_qQ \).
Splines on shape spaces

We introduce a forcing term $u$ as:

\[
\begin{align*}
\dot{p}_t &= -\partial_q H(p_t, q_t) + u_t \\
\dot{q}_t &= \partial_p H(p_t, q_t)
\end{align*}
\] (10)

Definition (Shape Splines)

Shape splines are defined as minimizer of the following functional:

\[
\inf_u J(u) = \frac{1}{2} \int_0^T \|u_t\|^2_X dt + \sum_{j=1}^k |q_{t_j} - x_{t_j}|^2.
\] (11)

subject to \((p, q)\) perturbed geodesic through $u_t$ for a freely chosen norm $\|\cdot\|_X$ on $T^*q$. 
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\]  

(11)

*subject to $(q, p)$ perturbed geodesic through $u_t$ for a freely chosen norm $\| \cdot \|_X$ on $T_q^*$.***
Simulations

Figure: Comparison between piecewise geodesic interpolation and spline interpolation
Simulations

Figure: Comparison between piecewise geodesic interpolation and spline interpolation

- Matching of 4 timepoints from an initial template.
- $|\cdot|_X$ is the Euclidean metric.
- Smooth interpolation in time.
Information contained in the acceleration and extrapolation

Figure: 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.
Robustness to noise

Due to the spatial regularisation of the kernel:

Figure: Gaussian noise added to the position of 50 landmarks
Robustness to noise

Due to the spatial regularisation of the kernel:

- Left: no noise.
- Center: standard deviation of 0.02.
- Right: standard deviation of 0.09.

**Figure**: Gaussian noise added to the position of 50 landmarks
Stochastics
A stochastic model:

Theorem

If \( k \) is \( C^1 \), the solutions of the stochastic differential equation defined by

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

are non exploding with few assumptions on \( u_t \) and \( \varepsilon \).
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\end{align*}
\]

(12)

are non exploding with few assumptions on $u_t$ and $\varepsilon$.

**Figure:** 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.
Simple PCA on the forcing term

Figure: Top row: Four examples of time evolution reconstructions from the observations 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 evolutions from the PCA analysis are visually good.
Ongoing work

- Extension to infinite dimensions (diffeomorphism group and images)
- Spline regression on the space of real images and statistical studies.
Geodesic regression

Enforcing the geodesicity constraint, shooting methods on the space of images:

\[
S(P(0)) = \frac{\lambda}{2} \langle \nabla I(0)P(0), K \ast \nabla I(0)P(0) \rangle_{L^2} + \frac{1}{2} \| I(1) - J \|^2_{L^2}.
\]  

(13)

with:

\[
\begin{cases}
\partial_t I + v \cdot \nabla I = 0, \\
\partial_t P + \nabla \cdot (vP) = 0, \\
v + K \ast (P \nabla I) = 0.
\end{cases}
\]

(14)
Adjoint equations

Proposition

The gradient of $S$ is given by:
$$\nabla_{P(0)} S = -\hat{P}(0) + \nabla I(0) \cdot K \ast (P(0) \nabla I(0))$$
where $\hat{P}(0)$ is given by the solution the backward PDE in time:

$$\begin{align*}
\partial_t \hat{I} + \nabla \cdot (\nu \hat{I}) + \nabla \cdot (P \hat{v}) &= 0, \\
\partial_t \hat{P} + v \cdot \nabla \hat{P} - \nabla I \cdot \hat{v} &= 0, \\
\hat{v} + K \ast (\hat{I} \nabla I - P \nabla \hat{P}) &= 0,
\end{align*}$$

subject to the initial conditions:

$$\begin{align*}
\hat{I}(1) &= J - I(1), \\
\hat{P}(1) &= 0,
\end{align*}$$

(15)

(16)
A key point: Integral formulation
Gradient descent based on an integral formulation:

**Theorem**

Let $I(0), J \in H^2(\Omega, \mathbb{R})$ be two images and $K$ be a $C^2$ kernel on $\Omega$. For any $P(0) \in L^2(\Omega)$, let $(I, P)$ be the solution of the shooting equations with initial conditions $I(0), P(0)$. Then, the corresponding adjoint equations have a unique solution $(\hat{I}, \hat{P})$ in $C^0([0, 1], H^1(\Omega) \times H^1(\Omega))$ such that

\[
\begin{align*}
\hat{P}(t) &= \hat{P}(1) \circ \phi_{t,1} - \int_t^1 [\nabla I(s) \cdot \hat{v}(s)] \circ \phi_{t,s} \, ds, \\
\hat{I}(t) &= \text{Jac}(\phi_{t,1})\hat{I}(1) \circ \phi_{t,1} \\
&\quad + \int_t^1 \text{Jac}(\phi_{t,s})[\nabla \cdot (P(s)\hat{v}(s))] \circ \phi_{t,s} \, ds.
\end{align*}
\]

with:

\[
\begin{align*}
\hat{v}(t) &= K * [P(t)\nabla \hat{P}(t) - \hat{I}(t)\nabla I(t)], \\
P(t) &= \text{Jac}(\phi_{t,0})P(0) \circ \phi_{t,0}, \\
I(t) &= I(0) \circ \phi_{t,0},
\end{align*}
\]

(18)

where $\phi_{s,t}$ is the flow of $v(t) = -K * P(t)\nabla I(t)$. 
Numerical examples on points

Figure:
- First Column: Geodesic Regression
- Second column: Linear Interpolation
- Third Column: Spline Interpolation
I warmly thank Colin Cotter, Darryl Holm, David Meier, Marc Niethammer, Laurent Risser and Alain Trouvé for this work.

- Shape Splines and Stochastic Shape Evolutions: A Second-Order Point of View. QAM (Trouvé A. and Vialard F.X.)