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HIGH ORDER SMOOTHING SPLINES *VERSUS* LEAST SQUARES PROBLEMS ON RIEMANNIAN MANIFOLDS

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ABSTRACT: In this paper, we present a generalization of the classical least squares problem on Euclidean spaces, introduced by Lagrange, to more general Riemannian manifolds. Using the variational definition of Riemannian polynomials, we formulate a high order variational problem on a manifold equipped with a Riemannian metric, which depends on a smoothing parameter and gives rise to what we call smoothing geometric splines. These are curves with a certain degree of smoothness that best fit a given set of points at given instants of time and reduce to Riemannian polynomials when restricted to each subinterval.

We show that the Riemannian mean of the given points is achieved as a limiting process of the above. Also, when the Riemannian manifold is an Euclidean space, our approach generates, in the limit, the unique polynomial curve which is the solution of the classical least squares problem. These results support our belief that the approach presented in this paper is the natural generalization of the classical least squares problem to Riemannian manifolds.

KEYWORDS: Riemannian manifolds, smoothing splines, Lie groups, least square problems, geometric polynomials.

1. Introduction

Curve fitting techniques on Euclidean spaces are well known in the literature, being the classical least squares problems the most common [21]. In these methods, introduced by Lagrange, we are given a finite set of points and a sequence of times with the objective to find a polynomial curve that best fits the given data.

Nevertheless, most part of the mechanical systems that appear in modern applications have components that are manifolds such as Lie groups or symmetric spaces, and more general fitting techniques have been required. This is the case, for instance, in the trajectory planning problem arising in robotics, aeronautics and air traffic control.

One of the main difficulties encountered in establishing the generalization of these standard fitting techniques has been the lack of the analogues to polynomial curves in Riemannian manifolds. This obstacle was overcome about two decades ago, when Noakes, Heinzinger and Paden [27], similarly to what

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happens in Euclidean spaces [13], defined cubic polynomials on manifolds as being curves that minimize the squared norm of the covariant acceleration. Following this variational approach, Camarinha et al. [5], on their work on higher order interpolating splines on non-Euclidean spaces, also defined high order Riemannian polynomials. In these two papers, Riemannian polynomials were defined as solutions of the Euler-Lagrange equations associated with certain variational problems.

However, due to the high nonlinearity of these differential equations, explicit solutions for Riemannian polynomials are extremely hard to find, except for some trivial cases. In spite of the effort spent by several authors using different perspectives, many questions remain open. We mention [10], [4], [8], [14], [19], [6] for an account of important theoretical contributions in this area. Equally important results for some particular manifolds with strong connections to applications are, for instance, [1], [7], [34], [20], [2].

As an attempt to overcome issues related to the computation of Riemannian polynomials, other alternative approaches have been proposed. One is based on a geometric construction called the De Casteljau algorithm [11], [13]. This algorithm was generalized for Riemannian manifolds [28], [8], [29] and several of the difficulties encountered with the variational approach have been overcome. Unfortunately, this alternative was not capable of producing explicit formulas for geometric splines even for low dimensional manifolds.

Under the above considerations and inspired by the definition of geometric polynomials on curved spaces, we propose here a natural generalization of the classical least squares problem to Riemannian manifolds. Such generalization is based in the formulation of a high order variational problem, depending on a smoothing parameter, whose solutions are smoothing curves minimizing the L^2-norm of the covariant derivative of order $m \geq 1$, that fit a given data set of points at given times. Solutions are called for that reason *smoothing geometric splines*. This approach follows the ideas behind the construction of smoothing splines for the S^2 sphere encountered in [17] and generalizes our previous work [24], where only the case $m = 2$ was treated.

Here, we establish and prove the necessary optimality conditions for the proposed variational problem and show that the Riemannian mean of the given points is obtained as a limiting process for the particular case when $m = 1$. This result extends to more general Riemannian manifolds what was done in [23] for compact and connected Lie groups and spheres.

Also, when the manifold is an Euclidean space and the smoothing parameter goes to infinity, the smoothing geometric splines converge to the solution of the classical least squares problem. This fact supports our strong belief that this is the natural generalization of the classical least squares problem to Riemannian manifolds.

Interpolating splines (studied, for instance, in [27], [9], [10], [5] and [15]) also arise as a limiting process of the above variational problems. However, in many applications it is not really crucial to pass through the given points exactly, but rather to go reasonably close to them. This is the case when a small deviation from the given points can result in a significant decrease of the cost. Another realistic situation arises when we are working with data which stems from experimental tasks and is corrupted by noise, situations that frequently occur in data analysis and statistics [33].

The outline of the paper is as follows. In section 2, we gather all the background from differential geometry needed throughout the paper. In section 3, we formulate the variational problem, state and prove the necessary optimality conditions for this problem. We also study the particular case of broken geodesics and prove that the Riemannian mean arises as a limiting process. Finally, in section 4 we recall the classical least squares problem in Euclidean spaces and prove that its solution is in fact achieved as a limiting process of the variational problem formulated in section 3. We also show in simulations, for some particular manifolds and some special data that our approach works in practice as well as in theory.

2. Preliminaries

In what follows, M denotes an $n-$dimensional Riemannian manifold endowed with the Levi-Civita connection denoted by ∇. Given $p \in M$, T_pM denotes the tangent space of M at p and $\langle \cdot, \cdot \rangle$ represents the inner product in T_pM. TM stands for the tangent bundle of M.

A vector field V along a curve $c : I \subset \mathbb{R} \to M$ is a mapping that assigns to each $t \in I$, the vector $V(t) \in T_{c(t)}M$. The velocity vector field of c, that we denote by $\dfrac{dc}{dt}$, is an example of a vector field. If V is induced by some vector field $X : M \to TM$, that is, if $V(t) = X_{c(t)}$, then we define the covariant derivative of V along c as being

$$\frac{DV}{dt} = \nabla_{\frac{dc}{dt}} X. \tag{2.1}$$

More generally, we have

$$\frac{D^m V}{dt^m} = \frac{D^{m-1}}{dt^{m-1}}\Big(\frac{DV}{dt}\Big), \ \ \forall\, m \geq 2.$$

The Levi-Civita connection ∇ is the unique affine connection that is compatible with the Riemannian metric and therefore, if V and W are smooth vector fields along a curve c, then

$$\frac{d}{dt}\Big\langle V, W\Big\rangle = \Big\langle \frac{DV}{dt}, W\Big\rangle + \Big\langle V, \frac{DW}{dt}\Big\rangle. \tag{2.2}$$

The previous equality can be seen as a particular case of the more general property that is stated by the following lemma.

Lemma 2.1. [5]

$$\Big\langle \frac{D^p V}{dt^p}, \frac{D^q W}{dt^q}\Big\rangle = \sum_{l=1}^{p} (-1)^{l-1}\frac{d}{dt}\Big\langle \frac{D^{p-l}V}{dt^{p-l}}, \frac{D^{q+l-1}W}{dt^{q+l-1}}\Big\rangle + (-1)^p\Big\langle V, \frac{D^{p+q}W}{dt^{p+q}}\Big\rangle,$$

where $p, q \in \mathbb{N}_0$.

A vector field V along a curve c is said to be parallel if

$$\frac{DV}{dt} = 0. \tag{2.3}$$

Taking into account the existence and uniqueness theorem for ordinary differential equations, it can be easily seen that given $V_0 \in T_{c(0)}M$, there exists a unique parallel vector field V along c such that $V(0) = V_0$. This vector field is called the parallel translate of V_0 along c. Thus, we can establish a linear isomorphism between tangent spaces, called the *parallel transport*,

$$\begin{array}{rrcl} P_{0,t}: & T_{c(0)}M & \longrightarrow & T_{c(t)}M \\ & V_0 & \longmapsto & P_{0,t}\big(V_0\big) = V(t) \end{array},$$

being $V(t)$ the unique parallel translate of V_0 along c.

By definition, a geodesic c is a smooth curve whose velocity vector is a parallel vector field along c. That is,

$$\frac{D}{dt}\Big(\frac{dc}{dt}\Big) = 0.$$

The above condition can also be written as $\dfrac{D^2 c}{dt^2} = 0$.

Therefore, according to the theory of existence and uniqueness for ordinary differential equations, given $p \in M$ and $v \in T_pM$, there is a unique geodesic $c : [0,1] \to M$, satisfying $c(0) = p$ and $\dfrac{dc}{dt}(0) = v$.

$c(1)$ is the point in the geodesic that is at a distance equal to $\|v\|$ from p and is denoted by $\exp_p(v)$, [25].

Therefore c is a constant speed curve that can be parameterized explicitly by

$$c(t) = \exp_p(tv).$$

Although, in general, the exponential map is only a terminology, there are some special Riemannian manifolds where it can be explicitly defined. In Euclidean spaces, geodesics are the straight lines and therefore, the exponential map is simply given by

$$\exp_p(tv) = p + tv.$$

For the unit sphere S^n, equipped with the Riemannian metric from the embedded space, geodesics are the great circles, and therefore,

$$\exp_p(tv) = p\cos\big(t\|v\|\big) + \frac{v}{\|v\|}\sin\big(t\|v\|\big). \tag{2.4}$$

For the case of connected and compact Lie groups, endowed with the bi-invariant Riemannian metric, geodesics through a point p are translations of 1-parameter subgroups, i.e.,

$$\exp_p(tv) = p\,\mathrm{e}^{tv}, \tag{2.5}$$

where e^{tv} stands for the sum of the power series $\mathrm{e}^{tv} = \displaystyle\sum_{m=0}^{+\infty} \frac{t^m v^m}{m!}$.

Since $v = \dfrac{dc}{dt}(0) \in T_{c(0)}M$, using the definition of parallel transport given above, it follows that

$$P_{0,t}(v) = \frac{dc}{dt}(t).$$

When every two points in M can be joined by a unique minimizing geodesic, we say that M is geodesically complete.

Following [18], the unique minimizing geodesic from p to q can be parameterized explicitly by

$$c(s) = \exp_p\big(s\exp_p^{-1}(q)\big), \quad s \in \big[0,1\big]. \tag{2.6}$$

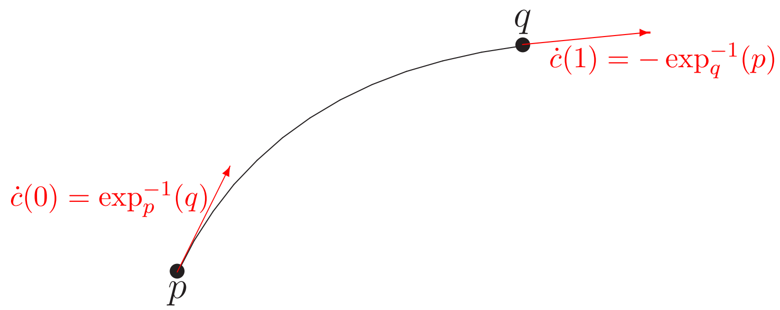

FIGURE 1. The minimizing geodesic joining p to q.

In this case, the distance between p and q is, therefore,

$$d(p,q) = \Big\langle \exp_p^{-1}(q), \exp_p^{-1}(q) \Big\rangle^{\frac{1}{2}},$$

and M becomes a complete metric space when endowed with the metric induced by the distance function.

A subset $C \subset M$ is said to be geodesically convex if any two points in C can be joined by a minimizing geodesic in M that lies entirely in C, [12].

Keeping the terminology of do Carmo [12], we adopt the following definition for the curvature tensor in M:

$$R(X,Y)Z = \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z + \nabla_{[X,Y]} Z,$$

where X, Y and Z are smooth vector fields in M.

The curvature tensor satisfies several symmetry relations that will be used throughout the paper and are listed below.

Lemma 2.2. [25] *If X, Y, Z and W are smooth vector fields, the curvature tensor R satisfies the following symmetry relations:*

1. $R(X,Y)Z = -R(Y,X)Z$;
2. $R(X,Y)Z + R(Y,Z)X + R(Z,X)Y = 0$;
3. $\big\langle R(X,Y)Z, W \big\rangle = -\big\langle R(X,Y)W, Z \big\rangle$;
4. $\big\langle R(X,Y)Z, W \big\rangle = \big\langle R(W,Z)Y, X \big\rangle$.

Also, given a point $p \in M$, and a two dimensional subspace Ξ of T_pM, if $\big\{X, Y\big\}$ is any basis of Ξ, the real number

$$\Delta(\Xi) = \frac{\Big\langle R(X,Y)Y, X \Big\rangle}{\sqrt{\|X\|^2 \|Y\|^2 - \langle X, Y \rangle^2}},$$

denotes the sectional curvature of Ξ at p.

Now, let $\alpha : (x, y) \in \mathbb{R}^2 \mapsto \alpha(x, y) \in M$ be a smooth parameterized surface in M. In spite of the following symmetry condition (do Carmo [12])

$$\frac{D}{\partial x}\Big(\frac{\partial \alpha}{\partial y}\Big) = \frac{D}{\partial y}\Big(\frac{\partial \alpha}{\partial x}\Big), \tag{2.7}$$

the two covariant differentiation operators $\dfrac{D}{\partial y}$ and $\dfrac{D}{\partial y}$ do not commute in general. The extent of noncommutativity of these two operators is given by the curvature tensor as it is shown in the next lemma.

Lemma 2.3. [25] *If V is a vector field along the parameterized surface α, then*

$$\frac{D}{\partial y}\frac{D}{\partial x}V = \frac{D}{\partial x}\frac{D}{\partial y}V + R\Big(\frac{\partial \alpha}{\partial y}, \frac{\partial \alpha}{\partial x}\Big)V. \tag{2.8}$$

Using high order covariant differentiation, a more general result was established in [5], as follows.

Proposition 2.4.

$$\frac{D}{\partial y}\Big(\frac{D^m V}{\partial x^m}\Big) = \frac{D^m}{\partial x^m}\Big(\frac{DV}{\partial y}\Big) + \sum_{j=2}^{m} \frac{D^{m-j}}{\partial t^{m-j}} R\Big(\frac{\partial \alpha}{\partial y}, \frac{\partial \alpha}{\partial x}\Big)\frac{D^{j-1}\alpha}{\partial x^{j-1}}. \tag{2.9}$$

2.1. Riemannian Mean. In Euclidean spaces there are several concepts of means [26], each of them with numerous applications in different areas. Nevertheless, the most common is indeed the arithmetic mean, also know as the center of mass, centroid or barycenter. For the set of points $p_0, \ldots, p_N$, belonging to the Euclidean space $\mathbb{R}^n$, it is simply defined as

$$\bar{p} = \frac{1}{N+1}\sum_{i=0}^{N} p_i. \tag{2.10}$$

The above formula has not a straightforward generalization to more general Riemannian manifolds, unless we notice that the arithmetic mean (2.10) is the unique solution of the following minimization problem:

$$\min_{p \in \mathbb{R}^n} \sum_{i=0}^{N} \big\|p - p_i\big\|^2.$$

That is, $\bar{p}$ minimizes the sum of the squared Euclidean distances from a point p to each p_i.

Now, a natural generalization of the above formulation to a Riemannian manifold M, consists in replacing the Euclidean distance by the geodesic distance. The Riemannian mean of the points $p_0, \ldots, p_N$ lying in M, is defined as being the set of points $p \in M$ that yield the minimum value for the function

$$\Phi(p) = \sum_{i=0}^{N} d^2(p, p_i). \tag{2.11}$$

It has been already proved in the literature ([18]), that a necessary condition for $p \in M$ to be a local minimum for Φ is that

$$\sum_{i=0}^{N} \exp_p^{-1}(p_i) = 0. \tag{2.12}$$

Contrary to what happens in Euclidean spaces, we have no guarantee that the Riemannian mean of a set of points is unique. If we think of two antipodal points on the sphere S^2, it is easy to check that all the points lying in the equator yield the minimum value for the function (2.11).

However, when the points are sufficiently close, it has been proved, in Karcher [18], that the Riemannian mean of the given points is unique.

Theorem 2.5. [18] *If B_ρ is a convex geodesic ball in M, with radius $\rho < \frac{\pi}{4}\Delta^{-\frac{1}{2}}$, being $\Delta > 0$ the maximum value of the sectional curvature in B_ρ, then function Φ is convex in B_ρ and it has a unique point of local minimum in B_ρ.*

The above result has been already extended by several authors for some particular symmetric spaces, like for instance, the Lie group of rotations [19], [16], and the unit $n-$sphere [3].

In this paper, we present an alternative way to obtain the Riemannian mean of a given set of points in M, based on the solution of a variational problem that gives rise to broken geodesics fitting those points.

2.2. High Order Polynomials on Riemannian Manifolds. Polynomials on Euclidean spaces are well behaviored curves that have a wide range of applications. Actually, interpolating splines based on cubic polynomials are the most used in approximation theory and the classical least squares problems introduced by Lagrange (1736-1813), also based in Euclidean polynomials, are a typical tool in the context of fitting curves.

Since our main objective here is to establish the generalization of the classical least squares problems to more general Riemannian manifolds, the first step is to recall how to define polynomials on manifolds.

About two decades ago, cubic polynomials on Riemannian manifolds have been introduced by Noakes, Heinzinger and Paden [27], as being extremal curves for the functional

$$L_2(\gamma) = \frac{1}{2}\int_0^T \Big\langle \frac{D^2\gamma}{dt^2}, \frac{D^2\gamma}{dt^2} \Big\rangle \, dt,$$

over an appropriate family of smooth curves $\gamma : [0, T] \to M$, satisfying some prescribed boundary conditions.

Analogously to what happens in Euclidean spaces [13], cubic polynomials on Riemannian manifolds also minimize changes in the acceleration, but only that component that is tangent to the manifold.

Later on, high order polynomials on Riemannian manifolds, also known as geometric polynomials, have been introduced in the literature by Camarinha et al. [5], as a generalization of the above and have been defined as the extremals for the functional

$$L_m(\gamma) = \frac{1}{2}\int_0^T \Big\langle \frac{D^m\gamma}{dt^m}, \frac{D^m\gamma}{dt^m} \Big\rangle \, dt, \tag{2.13}$$

over an appropriate family of curves.

Due to difficulties in characterizing properties and finding explicit solutions for this variational problem other notions of Riemannian polynomials have been introduced in the literature. For instance, the De Casteljau algorithm in Euclidean spaces produces curves that coincide with the solutions of the variational approach, but its generalization to Riemannian manifolds does not ([8]). However, we adopt the definition of Camarinha et al. [5], and define a Riemannian polynomial of degree $2m-1$ as the solutions of the Euler-Lagrange equations associated to 2.13. That is,

$$\frac{D^{2m}\gamma}{dt^{2m}} + \sum_{j=2}^{m} (-1)^j R\Big(\frac{D^{2m-j}\gamma}{dt^{2m-j}}, \frac{D^{j-1}\gamma}{dt^{j-1}}\Big)\frac{d\gamma}{dt} = 0. \tag{2.14}$$

Cubic polynomials are therefore obtained by considering $m = 2$ in (2.14), and are, therefore solutions of

$$\frac{D^4\gamma}{dt^4} + R\Big(\frac{D^2\gamma}{dt^2}, \frac{d\gamma}{dt}\Big)\frac{d\gamma}{dt} = 0.$$

Even in this case, the differential equation is highly non-linear and many questions concerning the geometry and ways to compute its solution remain open, in spite of the effort taken by several researchers using different perspectives. For more details, we mention [27], [4], [9], [10], [31], [6], [14], [29], and the references therein.

In the next lemma, we define an invariant along a geometric polynomial. This invariant was derived independently in [22] and in [29], and will be useful to prove some of the results appearing in the next section.

Lemma 2.6. *The quantity*

$$I = \sum_{j=1}^{m-1} (-1)^{j-1} \Big\langle \frac{D^{2m-j}\gamma}{dt^{2m-j}}, \frac{D^j\gamma}{dt^j} \Big\rangle + \frac{(-1)^{m-1}}{2} \Big\langle \frac{D^m\gamma}{dt^m}, \frac{D^m\gamma}{dt^m} \Big\rangle, \tag{2.15}$$

is preserved along a smooth curve satisfying (2.14)*.*

For the particular case when $m = 2$, the invariant (2.15) reduces to the invariant along a cubic polynomial derived in Camarinha et al. [6].

Lemma 2.7. *If the invariant* (2.15) *vanishes identically along the geometric polynomial* (2.14)*, then*

$$\sum_{j=1}^{m-1} (-1)^{j-1} j \frac{d}{dt} \Big\langle \frac{D^{2m-j}\gamma}{dt^{2m-j}}, \frac{D^{j-1}\gamma}{dt^{j-1}} \Big\rangle = (-1)^m \Big(m - \frac{1}{2}\Big) \Big\langle \frac{D^m\gamma}{dt^m}, \frac{D^m\gamma}{dt^m} \Big\rangle. \tag{2.16}$$

3. Problem's Statement

Let us start with a given set of points in M, $p_0, p_1, \ldots, p_N$, and a set of instants of time $0 = t_0 < t_1 < \cdots < t_N = 1$.

By Ω we denote the set of all C^{m-1} paths $\gamma : [0,1] \to M$ such that $\gamma\Big|_{[t_i,t_{i+1}]}$ is smooth (C^∞) and therefore both the limits $\lim\limits_{x\to t_i^+} \frac{D^k\gamma}{dt^k}(t)$ and $\lim\limits_{x\to t_{i+1}^-} \frac{D^k\gamma}{dt^k}(t)$ are bounded, for all $k \in \mathbb{N}$.

We define the tangent space of Ω at a path γ, $T_\gamma\Omega$, as being the set of all C^{m-1} vector fields $W : [0,1] \to TM$ such that $W\Big|_{[t_i,t_{i+1}]}$ is smooth.

Hereafter, we use the notation $\gamma \in C^k\big[a,b\big]$ to mean that the curve γ is of class C^k in the interval $\big[a,b\big]$.

Let us consider the following variational problem

$$(\mathcal{P}) \qquad \min_{\gamma\in\Omega} J(\gamma) = \frac{1}{2}\sum_{i=0}^{N} d^2\big(p_i, \gamma(t_i)\big) + \frac{\lambda}{2}\int_0^1 \langle \frac{D^m\gamma}{dt^m}, \frac{D^m\gamma}{dt^m}\rangle \, dt,$$

where λ denotes a positive real number that will play the role of a smoothing parameter, as will be seen sooner.

Notice that

$$J(\gamma) = E(\gamma) + \lambda L_m(\gamma),$$

where

$$E(\gamma) = \frac{1}{2}\sum_{i=0}^{N} d^2\big(p_i, \gamma(t_i)\big),$$

and L_m is defined by (2.13).

Since γ is an extremal for the functional J if and only its first variation vanishes for all variations of γ, we need to compute the first variation of J,

$$\frac{\partial}{\partial u}\Big|_{u=0} J\big(\alpha(u,t)\big), \tag{3.17}$$

where $\alpha : \big]-\varepsilon, \varepsilon\big[\times \big[0,1\big] \longmapsto \alpha(u,t) \in M$ is a variation of γ.

Variations may be defined as

$$\alpha(u,t) = \exp_{\gamma(t)}\big(uW(t)\big), \tag{3.18}$$

where $W : \big[0,1\big] \to TM$ is a variation vector field along γ lying in $T_\gamma\Omega$. Therefore,

$$W(t) = \frac{\partial\alpha}{\partial u}(0,t).$$

Since,

$$\frac{\partial}{\partial u}\Big|_{u=0} J\big(\alpha(u,t)\big) = \frac{\partial}{\partial u}\Big|_{u=0} E\big(\alpha(u,t)\big) + \lambda\frac{\partial}{\partial u}\Big|_{u=0} L\big(\alpha(u,t)\big),$$

we start with the computation of $\frac{\partial}{\partial u}\Big|_{u=0} E\big(\alpha(u,t)\big)$.

For each $i = 0, \ldots, N$, let us denote by

$$c_i(s) = \exp_{p_i}\big(s\exp_{p_i}^{-1}\big(\gamma(t_i)\big)\big), \tag{3.19}$$

the minimal geodesic joining the point p_i (at $s = 0$) to the point $\gamma(t_i)$ (at $s = 1$).

Introducing, in (3.19), the variation α defined by (3.18), we obtain the parameterized surface in M, $c_i : [0,1] \times]-\varepsilon, \varepsilon[\longrightarrow M$, given by

$$c_i(s,u) = \exp_{p_i}\big(s \exp_{p_i}^{-1}(\alpha(u,t_i))\big).$$

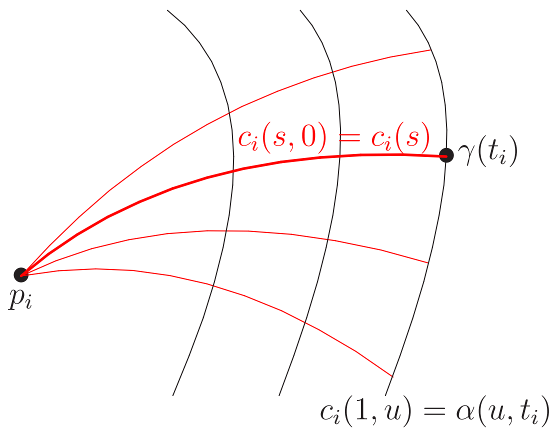

FIGURE 2. The parameterized surface c_i.

Therefore, we can define two family of curves

$$s \longmapsto c_i(s,u),$$

by setting u constant, and

$$u \longmapsto c_i(s,u),$$

by setting s constant, and, consequently, two family of vector fields

$$S_i(s,u) = \frac{\partial c_i}{\partial s}(s,u),$$

and,

$$U_i(s,u) = \frac{\partial c_i}{\partial u}(s,u).$$

Since, for each fixed u, $s \longmapsto c_i(s,u)$ is a geodesic, S_i is a parallel vector field along that geodesic, i.e.,

$$\frac{DS_i}{\partial s}(s,u) = 0.$$

On the other hand, there exists a unique minimizing geodesic joining p_i to $\alpha(u,t_i)$ (see figure 3), so we can write

$$d^2\big(p_i, \alpha(u,t_i)\big) = \Big\langle S_i(s,u), S_i(s,u) \Big\rangle = \int_0^1 \Big\langle S_i(s,u), S_i(s,u) \Big\rangle \, ds.$$

Now, using the symmetry condition (2.7) together with the compatibility condition (2.2), we can still write

$$\begin{aligned}
\frac{\partial}{\partial u}E\big(\alpha(u,t)\big) &= \sum_{i=0}^{N}\int_0^1 \Big\langle \frac{DS_i}{\partial u}(s,u), S_i(s,u)\Big\rangle\, ds \\
&= \sum_{i=0}^{N}\int_0^1 \Big\langle \frac{DU_i}{\partial s}(s,u), S_i(s,u)\Big\rangle\, ds \\
&= \sum_{i=0}^{N}\int_0^1 \frac{\partial}{\partial s}\Big\langle U_i(s,u), S_i(s,u)\Big\rangle\, ds \\
&= \sum_{i=0}^{N}\Big\langle U_i(1,u), S_i(1,u)\Big\rangle - \Big\langle U_i(0,u), S_i(0,u)\Big\rangle.
\end{aligned}$$

By setting $u=0$, and taking into account that $S_i(1,0) = -\exp^{-1}_{\gamma(t_i)}(p_i)^*$, we get

$$\frac{\partial}{\partial u}\Big|_{u=0} E\big(\alpha(u,t)\big) = -\sum_{i=0}^{N}\Big\langle W(t_i), \exp^{-1}_{\gamma(t_i)}(p_i)\Big\rangle. \tag{3.20}$$

It remains to derive the first variation of functional L. In this case, we will use lemma 2.1 and proposition 2.4 and follow analogous steps to those in [5],

*Notice that $c_i(s,0)$ is the minimizing geodesic joining p_i to $\gamma(t_i)$ and recall figure 1.

adapted to the current situation.

$$
\begin{aligned}
&\frac{\partial}{\partial u} L\big(\alpha(u,t)\big) = \\
&= \int_0^1 \Big\langle \frac{D}{\partial u}\Big(\frac{D^m\alpha}{\partial t^m}\Big), \frac{D^m\alpha}{\partial t^m}\Big\rangle\, dt \\
&= \int_0^1 \Big\langle \frac{D^m}{\partial t^m}\Big(\frac{\partial\alpha}{\partial u}\Big), \frac{D^m\alpha}{\partial t^m}\Big\rangle\, dt + \sum_{j=2}^{m} \int_0^1 \Big\langle \frac{D^{m-j}}{\partial t^{m-j}} R\Big(\frac{\partial\alpha}{\partial u}, \frac{\partial\alpha}{\partial t}\Big)\frac{D^{j-1}\alpha}{\partial t^{j-1}}, \frac{D^m\alpha}{\partial t^m}\Big\rangle\, dt \\
&= \sum_{l=1}^{m} (-1)^{l-1} \int_0^1 \frac{\partial}{\partial t}\Big\langle \frac{D^{m-l}}{\partial t^{m-l}}\Big(\frac{\partial\alpha}{\partial u}\Big), \frac{D^{m+l-1}\alpha}{\partial t^{m+l-1}}\Big\rangle\, dt + (-1)^m \int_0^1 \Big\langle \frac{\partial\alpha}{\partial u}, \frac{D^{2m}\alpha}{\partial t^{2m}}\Big\rangle\, dt \\
&\quad + \sum_{j=2}^{m-1}\sum_{l=1}^{m-j} (-1)^{l-1} \int_0^1 \frac{\partial}{\partial t}\Big\langle \frac{D^{m-j-l}}{\partial t^{m-j-l}} R\Big(\frac{\partial\alpha}{\partial u}, \frac{\partial\alpha}{\partial t}\Big)\frac{D^{j-1}\alpha}{\partial t^{j-1}}, \frac{D^{m+l-1}\alpha}{\partial t^{m+l-1}}\Big\rangle\, dt \\
&\quad + \sum_{j=2}^{m} (-1)^{m-j} \int_0^1 \Big\langle R\Big(\frac{\partial\alpha}{\partial u}, \frac{\partial\alpha}{\partial t}\Big)\frac{D^{j-1}\alpha}{\partial t^{j-1}}, \frac{D^{2m-j}\alpha}{dt^{2m-j}}\Big\rangle\, dt.
\end{aligned}
$$

By letting $u = 0$ in the above expression and taking into account property 4 of the curvature tensor, listed in lemma 2.2, we get

$$
\begin{aligned}
&\frac{\partial}{\partial u}\Big|_{u=0} L\big(\alpha(u,t)\big) = \\
&= \sum_{l=1}^{m}\sum_{i=0}^{N-1} (-1)^{l-1} \Big\langle \frac{D^{m-l}W}{dt^{m-l}}, \frac{D^{m+l-1}\gamma}{dt^{m+l-1}}\Big\rangle\Big|_{t_i^+}^{t_{i+1}^-} \\
&\quad + \sum_{j=2}^{m-1}\sum_{l=1}^{m-j}\sum_{i=0}^{N-1} (-1)^{l-1} \Big\langle \frac{D^{m-j-l}}{dt^{m-j-l}} R\Big(W, \frac{d\gamma}{dt}\Big)\frac{D^{j-1}\gamma}{dt^{j-1}}, \frac{D^{m+l-1}\gamma}{dt^{m+l-1}}\Big\rangle\Big|_{t_i^+}^{t_{i+1}^-} \\
&\quad + (-1)^m \int_0^1 \Big\langle \frac{D^{2m}\gamma}{dt^{2m}} + \sum_{j=2}^{m} (-1)^j R\Big(\frac{D^{2m-j}\gamma}{dt^{2m-j}}, \frac{D^{j-1}\gamma}{dt^{j-1}}\Big)\frac{d\gamma}{dt}, W\Big\rangle\, dt
\end{aligned}
\tag{3.21}
$$

Putting together (3.20) and (3.21), we obtain the desired first variation of the functional J.

$$\begin{aligned}
&\frac{\partial}{\partial u}\Big|_{u=0} J\big(\alpha(u,t)\big) = \\
&= \sum_{l=1}^{m-1}\sum_{i=0}^{N}(-1)^l\lambda\Big\langle \frac{D^{m-l}W}{dt^{m-l}}(t_i), \frac{D^{m+l-1}\gamma}{dt^{m+l-1}}\big(t_i^+\big) - \frac{D^{m+l-1}\gamma}{dt^{m+l-1}}\big(t_i^-\big)\Big\rangle \\
&\quad + \sum_{i=0}^{N}\Big\langle W(t_i), (-1)^m\lambda\Big[\frac{D^{2m-1}\gamma}{dt^{2m-1}}\big(t_i^+\big) - \frac{D^{2m-1}\gamma}{dt^{2m-1}}\big(t_i^-\big)\Big] - \exp^{-1}_{\gamma(t_i)}(p_i)\Big\rangle \\
&\quad + \sum_{j=2}^{m-1}\sum_{l=1}^{m-j}\sum_{i=0}^{N-1}(-1)^{l-1}\lambda\Big\langle \frac{D^{m-j-l}}{dt^{m-j-l}}R\Big(W, \frac{d\gamma}{dt}\Big)\frac{D^{j-1}\gamma}{dt^{j-1}}, \frac{D^{m+l-1}\gamma}{dt^{m+l-1}}\Big\rangle\Big|_{t_i^+}^{t_{i+1}^-} \\
&\quad + (-1)^m\int_0^1 \lambda\Big\langle \frac{D^{2m}\gamma}{dt^{2m}} + \sum_{j=2}^{m}(-1)^j R\Big(\frac{D^{2m-j}\gamma}{dt^{2m-j}}, \frac{D^{j-1}\gamma}{dt^{j-1}}\Big)\frac{d\gamma}{dt}, W\Big\rangle\, dt.
\end{aligned} \tag{3.22}$$

We are now in a position to state and prove one of our main results.

Theorem 3.1. *A necessary condition for $\gamma \in \Omega$ to be a solution for problem $(\mathcal{P})$ is that $\gamma \in C^{2m-2}\big[0,1\big]$, satisfies for each $i = 0, \ldots N-1$, and $t \in \big[t_i, t_{i+1}\big]$, the differential equation*

$$\frac{D^{2m}\gamma}{dt^{2m}} + \sum_{j=2}^{m}(-1)^j R\Big(\frac{D^{2m-j}\gamma}{dt^{2m-j}}, \frac{D^{j-1}\gamma}{dt^{j-1}}\Big)\frac{d\gamma}{dt} = 0, \tag{3.23}$$

and at the knot points t_i, for $i = 0, \ldots, N$, it also satisfies the following conditions

$$\begin{cases} \dfrac{D^j\gamma}{dt^j}(t_i^+) - \dfrac{D^j\gamma}{dt^j}(t_i^-) = 0, & m \le j \le 2m-2 \\ \dfrac{D^{2m-1}\gamma}{dt^{2m-1}}(t_i^+) - \dfrac{D^{2m-1}\gamma}{dt^{2m-1}}(t_i^-) = \dfrac{(-1)^m}{\lambda}\exp^{-1}_{\gamma(t_i)}(p_i) \end{cases}, \tag{3.24}$$

where we assume for shorten of notation that $\dfrac{D^j\gamma}{dt^j}(t_0^-) = \dfrac{D^j\gamma}{dt^j}(t_N^+) = 0$, for $j = m, \ldots, 2m-1$.

Proof: In order for $\gamma \in \Omega$ to be an extremal for functional J, its first variation has to vanish for all variations α given by (3.18).

Let us consider a particular variation vector field W defined as

$$W(t) = (-1)^m F(t)\Big[\frac{D^{2m}\gamma}{dt^{2m}} + \sum_{j=2}^{m}(-1)^j R\Big(\frac{D^{2m-j}\gamma}{dt^{2m-j}}, \frac{D^{j-1}\gamma}{dt^{j-1}}\Big)\frac{d\gamma}{dt}\Big],$$

where $F : [0,1] \to \mathbb{R}$ is a positive piecewise smooth function satisfying, for each $i = 0, \ldots, N$,

$$F(t_i) = F'(t_i) = \cdots = F^{(m-1)}(t_i) = 0.$$

For this choice of the variation vector field W, we get from (3.22),

$$\frac{\partial}{\partial u}\Big|_{u=0} J\big(\alpha(u,t)\big) = \int_0^1 F(t)\Big\|\frac{D^{2m}\gamma}{dt^{2m}} + \sum_{j=2}^{m}(-1)^j R\Big(\frac{D^{2m-j}\gamma}{dt^{2m-j}}, \frac{D^{j-1}\gamma}{dt^{j-1}}\Big)\frac{d\gamma}{dt}, W\Big\|^2 dt.$$

Consequently, this vanishes identically if and only if, for each $i = 0, \ldots, N$, and $t \in \big[t_i, t_{i+1}\big]$,

$$\frac{D^{2m}\gamma}{dt^{2m}} + \sum_{j=2}^{m}(-1)^j R\Big(\frac{D^{2m-j}\gamma}{dt^{2m-j}}, \frac{D^{j-1}\gamma}{dt^{j-1}}\Big)\frac{d\gamma}{dt} = 0.$$

So, the first part of the statement is proved.

Now, if one considers a variation vector field W satisfying, for each $i = 0, \ldots, N$,

$$W(t_i) = \frac{DW}{dt}(t_i) = \cdots = \frac{D^{m-2}W}{dt^{m-2}}(t_i) = 0,$$

and

$$\frac{D^{m-1}W}{dt^{m-1}}(t_i) = \frac{D^m\gamma}{dt^m}(t_i^-) - \frac{D^m\gamma}{dt^m}(t_i^+),$$

we get

$$\frac{\partial}{\partial u}\Big|_{u=0} J\big(\alpha(u,t)\big) = \sum_{i=0}^{N} \lambda\Big\|\frac{D^m\gamma}{dt^m}(t_i^+) - \frac{D^m\gamma}{dt^m}(t_i^-)\Big\|^2,$$

which vanishes if and only if $\gamma \in C^m\big[0,1\big]$.

Now, if we choose a variation vector field W, such that for each $i = 0, \ldots, N$,

$$W(t_i) = \frac{DW}{dt}(t_i) = \cdots = \frac{D^{m-3}W}{dt^{m-3}}(t_i) = 0,$$

and

$$\frac{D^{m-2}W}{dt^{m-2}}(t_i) = \frac{D^{m+1}\gamma}{dt^{m+1}}(t_i^+) - \frac{D^{m+1}\gamma}{dt^{m+1}}(t_i^-),$$

it can easily be seen that if γ is a solution for problem $(\mathcal{P})$, then $\gamma \in C^{m+1}\big[0,1\big]$.

Proceeding analogously and choosing appropriate variation vector fields in a way similar to the last choice, we conclude that the requirement $\gamma \in C^{2m-2}\big[0,1\big]$ is necessary in order for γ to be an extremal for functional J.

Finally, choose the variation vector field W satisfying

$$W(t_i) = (-1)^m \lambda \Big[\frac{D^{2m-1}\gamma}{dt^{2m-1}}\big(t_i^+\big) - \frac{D^{2m-1}\gamma}{dt^{2m-1}}\big(t_i^-\big)\Big] - \exp^{-1}_{\gamma(t_i)}\big(p_i\big),$$

for each $i = 0, \ldots, N$, to conclude that, for this case,

$$\sum_{i=0}^{N} \Big\| (-1)^m \lambda \Big[\frac{D^{2m-1}\gamma}{dt^{2m-1}}\big(t_i^+\big) - \frac{D^{2m-1}\gamma}{dt^{2m-1}}\big(t_i^-\big)\Big] - \exp^{-1}_{\gamma(t_i)}\big(p_i\big)\Big\|^2 = 0,$$

and, therefore,

$$\frac{D^{2m-1}\gamma}{dt^{2m-1}}\big(t_i^+\big) - \frac{D^{2m-1}\gamma}{dt^{2m-1}}\big(t_i^-\big) = \frac{(-1)^m}{\lambda} \exp^{-1}_{\gamma(t_i)}\big(p_i\big).$$

This completes the proof. ∎

Remark 3.1. *From the above theorem, we can see that solutions for the variational problem* $(\mathcal{P})$ *are obtained by piecing together geometric polynomials of degree* $2m-1$ *in each subinterval* $\big[t_i, t_{i+1}\big]$*. According to the regularity conditions* (3.24)*, they fit the given points* p_i *at the given times* t_i*, this being the reason why we call them smoothing geometric splines.*

Proposition 3.2. [22] *Under conditions* (3.23)-(3.24) *of theorem* (3.1)*, the following holds.*

(a) *When* λ *goes to* 0*, then the smoothing geometric splines approach an interpolating spline that passes through each point* p_i *at each time* t_i*.*

(b) *When* λ *goes to* $+\infty$*, then the smoothing geometric splines approach a smooth curve in the whole interval* $[0,1]$ *fitting the given points at the given times, and satisfying the differential equation*

$$\frac{D^m\gamma}{dt^m} = 0. \tag{3.25}$$

Proof: Property (a) follows immediately if one multiplies both terms of the last equation in (3.24) by λ, and then take limits as λ goes to 0.

To prove property (b), take limits on both sides of (3.24), as λ goes to $+\infty$. In this case, the curve $\gamma \in C^{2m-1}\big[0,1\big]$, and satisfies

$$\frac{D^k\gamma}{dt^k}(0) = 0, \tag{3.26}$$

for $k = m, \ldots, 2m-1$.

According to the theory of ordinary differential equations, since γ belongs to $C^{2m-2}\big[0,1\big]$ and satisfies the differential equation (3.23) of order $2m$ in each subinterval $[t_i, t_{i+1}]$, it has to satisfy (3.23), for all $t \in [0,1]$.

Now, taking into account the boundary conditions (3.26), it is easy to see that the invariant I along the geometric polynomial γ, defined by (3.23) vanishes identically.

So, using lemma 2.7, we can conclude that the real function

$$t \longmapsto \sum_{j=1}^{m-1}(-1)^{j-1}j\Big\langle \frac{D^{2m-j}\gamma}{dt^{2m-j}}, \frac{D^{j-1}\gamma}{dt^{j-1}}\Big\rangle,$$

is a monotonous function in the interval $[0,1]$ (non-increasing for odd values of m and non-decreasing otherwise).

In both cases, according to the boundary conditions (3.26), the above function vanishes identically in $\big[0,1\big]$, and therefore,

$$\frac{D^m\gamma}{dt^m}(t) = 0, \quad \forall t \in [0,1].$$

■

Remark 3.2. *Smooth curves satisfying the differential equation* (3.25) *can be obtained by rolling (without slip or twist) a manifold on its affine tangent space* $T_{\gamma(0)}M$ *along an Euclidean polynomial of degree* $m-1$*, as it was shown recently in Silva Leite and Krakowski* [32].

The previous results show that for the particular case when $m = 1$ and the smoothing parameter λ goes to infinity in the system of equations (3.23)-(3.24), the smoothing geometric splines approach a single point. What we prove next is that this point turns out to be the Riemannian mean of the given points p_i, if we assume in advance that their Riemannian mean exists and is a singleton.

Theorem 3.3. *When* $m = 1$ *and* λ *goes to* $+\infty$ *in the conditions* (3.23)-(3.24), of theorem 3.1, then the smoothing geometric splines converge to the Riemannian mean of the given points p_i.

Proof: For $m = 1$, the differential equation (3.23) becomes

$$\frac{D^2\gamma}{dt^2} = 0, \tag{3.27}$$

and the regularity conditions (3.24) reduce simply to

$$\begin{aligned}
&\frac{d\gamma}{dt}(t_0^+) = -\frac{1}{\lambda}\exp^{-1}_{\gamma(t_0)}(p_0)\\
&\frac{d\gamma}{dt}(t_1^+) - \frac{d\gamma}{dt}(t_1^-) = -\frac{1}{\lambda}\exp^{-1}_{\gamma(t_1)}(p_1)\\
&\qquad\vdots\\
&\frac{d\gamma}{dt}(t_{N-1}^+) - \frac{d\gamma}{dt}(t_{N-1}^-) = -\frac{1}{\lambda}\exp^{-1}_{\gamma(t_{N-1})}(p_{N-1})\\
&\frac{d\gamma}{dt}(t_N^-) = \frac{1}{\lambda}\exp^{-1}_{\gamma(t_N)}(p_N)
\end{aligned} \quad . \tag{3.28}$$

Since γ is a geodesic in each subinterval $\big[t_i, t_{i+1}\big]$, let us denote by P_i the parallel transport along γ in that subinterval. This means that,

$$\frac{d\gamma}{dt}(t_{i+1}^-) = P_i\Big(\frac{d\gamma}{dt}(t_i^+)\Big), \tag{3.29}$$

and the regularity conditions (3.28) may be written as

$$\begin{aligned}
&\frac{d\gamma}{dt}(t_0^+) = -\frac{1}{\lambda}\exp^{-1}_{\gamma(t_0)}(p_0)\\
&\frac{d\gamma}{dt}(t_1^+) = -\frac{1}{\lambda}\exp^{-1}_{\gamma(t_1)}(p_1) - \frac{1}{\lambda}P_0\Big(\exp^{-1}_{\gamma(t_0)}(p_0)\Big)\\
&\quad\vdots\\
&\frac{d\gamma}{dt}(t_{N-1}^+) = -\frac{1}{\lambda}\exp^{-1}_{\gamma(t_{N-1})}(p_{N-1}) - \frac{1}{\lambda}P_{N-2}\Big(\exp^{-1}_{\gamma(t_{N-2})}(p_{N-2})\Big) - \cdots\\
&\qquad\qquad -\frac{1}{\lambda}\Big(P_{N-2}\circ P_{N-3}\circ\cdots\circ P_0\Big)\Big(\exp^{-1}_{\gamma(t_0)}(p_0)\Big)\\
&-\frac{1}{\lambda}P_{N-1}\Big(\exp^{-1}_{\gamma(t_{N-1})}(p_{N-1})\Big) - \frac{1}{\lambda}\Big(P_{N-1}\circ P_{N-2}\Big)\Big(\exp^{-1}_{\gamma(t_{N-2})}(p_{N-2})\Big) - \cdots\\
&-\frac{1}{\lambda}\Big(P_{N-1}\circ P_{N-2}\circ\cdots\circ P_0\Big)\Big(\exp^{-1}_{\gamma(t_0)}(p_0)\Big) = \frac{1}{\lambda}\exp^{-1}_{\gamma(t_N)}(p_N)
\end{aligned} \quad . \tag{3.30}$$

When λ goes to $+\infty$, it is clear from the above conditions that the broken geodesic γ reduces to a single point, say $\gamma(t) = p$, $\forall t \in [0, 1]$. Moreover, for each $i = 0, \ldots, N-1$, the parallel transport P_i degenerates into the identity map and the last equation in (3.30) becomes

$$\exp_p^{-1}(p_0) + \exp_p^{-1}(p_1) + \cdots + \exp_p^{-1}(p_N) = 0,$$

which proves that p is in fact the Riemannian mean of the points p_i. ■

In figures 3-6, we illustrate the previous result for some specific data and the particular cases when M is the Euclidean space $\mathbb{R}^2$ and the unit sphere S^2.

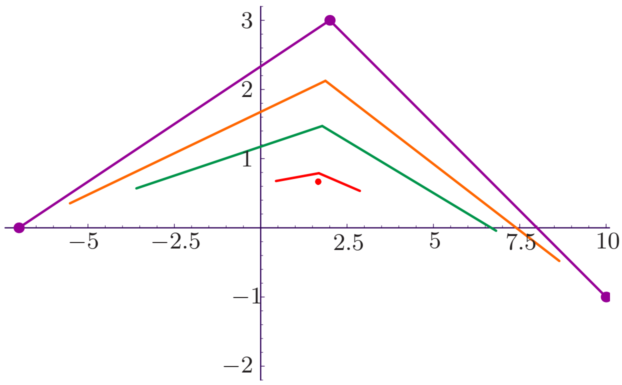

FIGURE 3. $q_0 = \big(-7, 0\big)$, $q_1 = (2, 3)$, $q_2 = (10, -1)$, $t_0 = 0$, $t_1 = \frac{1}{2}$ and $t_2 = 1$. The smoothing cubic splines were obtained for the following values of λ: $\lambda_1 = 10^{-5}$, $\lambda_2 = 10^{-1}$, $\lambda_3 = 10^{-0.5}$, $\lambda_4 = 3$ and $\lambda_5 = 10^3$.

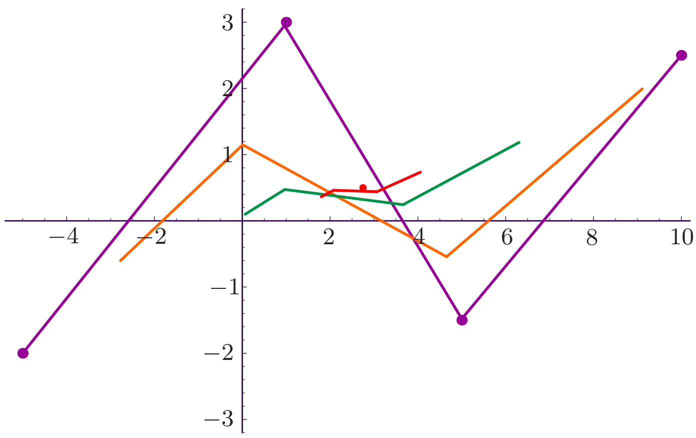

FIGURE 4. $q_0 = \big(-5, -2\big)$, $q_1 = (1, 3)$, $q_2 = \big(5, -\frac{3}{2}\big)$, $q_3 = \big(10, \frac{5}{2}\big)$, $t_0 = 0$, $t_1 = \frac{1}{8}$, $t_2 = \frac{1}{2}$ and $t_3 = 1$. The smoothing cubic splines were obtained for the following values of λ: $\lambda_1 = 10^{-3}$, $\lambda_2 = 10^{-1}$, $\lambda_3 = 0.7$, $\lambda_4 = 3$ and $\lambda_5 = 10^3$.

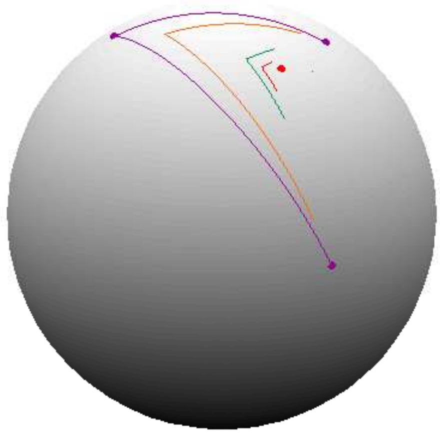

FIGURE 5. $q_0 = \left(\frac{\sqrt{2}}{4}, \frac{\sqrt{2}}{4}, \frac{\sqrt{3}}{2}\right)$, $q_1 = \left(-\frac{1}{4}, 0, \frac{\sqrt{3}}{2}\right)$, $q_2 = \left(1, 0, 0\right)$, $t_0 = 0$, $t_1 = \frac{1}{2}$ and $t_2 = 1$. The smoothing cubic splines were obtained for the following values of λ: $\lambda_1 = 10^{-3}$, $\lambda_2 = 10^{-1}$, $\lambda_3 = 1$, $\lambda_4 = 5$ and $\lambda_5 = 10^4$.

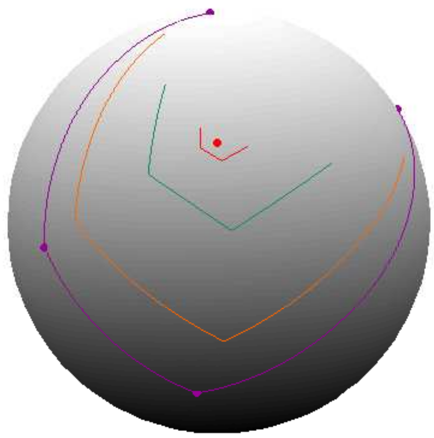

FIGURE 6. $q_0 = \left(0, 0, 1\right)$, $q_1 = (0, -1, 0)$, $q_2 = \left(\frac{1}{2}, -\frac{1}{2}, -\frac{\sqrt{2}}{2}\right)$, $q_3 = \left(\frac{\sqrt{3}}{4}, \frac{3}{4}, \frac{1}{2}\right)$, $t_0 = 0$, $t_1 = \frac{1}{3}$, $t_2 = \frac{2}{3}$ and $t_3 = 1$. The smoothing cubic splines were obtained for the following values of λ: $\lambda_1 = 10^{-4}$, $\lambda_2 = 10^{-1}$, $\lambda_3 = 0.5$, $\lambda_4 = 3$ and $\lambda_5 = 10^4$.

4. Smoothing Splines and Least Squares Problems

In this section, we will finally establish the relationship between the smoothing geometric splines defined in the previous section and the solution of the classical least squares problem in Euclidean spaces. The results that we develop throughout this section, which generalize the classical results appearing in [30] for the particular case when $m = 2$ and $M = \mathbb{R}^n$, strongly support our belief that the variational problem formulated at the very beginning of section 3 is the most natural way of generalizing the classical least squares problem to Riemannian manifolds.

Before we establish our main result of this section, we will briefly recall the classical least squares problem in Euclidean spaces.

4.1. Recalling the Classical Least Squares Problem. In the classical least squares problem, we are given a finite set of points in $\mathbb{R}^n$, $p_0, \ldots, p_N$, and an increasing sequence of instants of time $t_0 < \cdots < t_N$, and the objective is to find a polynomial curve $t \mapsto \gamma(t) = a_0 + a_1 t + \cdots + a_{m-1}t^{m-1}$, with $m-1 \leq N$, that minimizes the sum of the squared Euclidean distances from p_i to $\gamma(t_i)$. That is, that yields the minimum value for the functional

$$E(\gamma) = \sum_{i=0}^{N} \left\|p_i - \gamma(t_i)\right\|^2. \tag{4.31}$$

Although the classical literature only treats the case when the data belongs to $\mathbb{R}$, its generalization to more general Euclidean spaces is straightforward. In particular, it is easy to prove that the above problem has a unique solution γ, which is obtained by solving the following system of equations:

$$\begin{aligned} \sum_{i=0}^{N} \gamma(t_i) &= \sum_{i=0}^{N} p_i \\ \sum_{i=0}^{N} t_i\gamma(t_i) &= \sum_{i=0}^{N} t_i p_i \\ &\vdots \\ \sum_{i=0}^{N} t_i^{m-1}\gamma(t_i) &= \sum_{i=0}^{N} t_i^{m-1} p_i \end{aligned} \quad , \tag{4.32}$$

known in the literature as the normal equations [21].

4.2. Main Results. In what follows, we will assume that the Riemannian manifold M is the Euclidean space $\mathbb{R}^n$, endowed with the Riemannian metric induced by the Euclidean inner product.

Theorem 4.1. *When* $M = \mathbb{R}^n$ *and* λ *goes to* $+\infty$ *in conditions* (3.23)-(3.24) *of theorem* 3.1*, the smoothing splines converge to the polynomial of degree* $m-1$ *that is the solution of the classical least squares problem.*

Proof: For the case when M is the Euclidean space $\mathbb{R}^n$, the curvature tensor vanishes, the covariant derivative reduces to the usual derivative and therefore the differential equation (3.23) becomes simply

$$\frac{d^{2m}\gamma}{dt^{2m}} = 0. \tag{4.33}$$

The regularity conditions (3.24) take also the form

$$\begin{array}{l} \dfrac{d^k\gamma}{dt^k}(t_i^+) = \dfrac{d^k\gamma}{dt^k}(t_i^-) = 0, \qquad k = m, \ldots, 2m-2 \\ \dfrac{d^{2m-1}\gamma}{dt^{2m-1}}(t_i^+) - \dfrac{d^{2m-1}\gamma}{dt^{2m-1}}(t_i^-) = \dfrac{(-1)^m}{\lambda}\big(p_i - \gamma(t_i)\big) \end{array}, \tag{4.34}$$

for $i = 0, \ldots, N$.

Equation (4.33) can be integrate explicitly is each subinterval $\big[t_i, t_{i+1}\big]$. Let us consider

$$\gamma(t) = a_0^i + a_1^i t + \ldots + a_{2m-1}^i t^{2m-1}, \tag{4.35}$$

where $a_k^i \in \mathbb{R}^n$, for each $k = 0, \ldots, 2m-1$ and $i = 0, \ldots, N-1$.

Computing successively the derivatives of γ with respect to t, we get, for $t \in \big[t_i, t_{i+1}\big]$,

$$\begin{aligned} \frac{d\gamma}{dt}(t) &= a_1^i + 2a_2^i t + \cdots + (2m-1)a_{2m-1}^i t^{2m-2} \\ \frac{d^2\gamma}{dt^2}(t) &= 2a_2^i + 3!a_3^i t + \cdots + (2m-1)(2m-2)a_{2m-1}^i t^{2m-3} \\ &\vdots \\ \frac{d^k\gamma}{dt^k}(t) &= k!a_k^i + (k+1)!a_{k+1}^i t + \cdots + \frac{(2m-1)!}{(2m-k-1)!}a_{2m-1}^i t^{2m-k-1} \\ &\vdots \\ \frac{d^{2m-1}\gamma}{dt^{2m-1}}(t) &= (2m-1)!a_{2m-1}^i \end{aligned}.$$

Now, attending to the expression for the derivative of γ of order $2m-1$, it follows immediately that

$$\frac{d^{2m-1}\gamma}{dt^{2m-1}}\big(t_i^+\big) = \frac{d^{2m-1}\gamma}{dt^{2m-1}}\big(t_{i+1}^-\big), \tag{4.36}$$

where $i = 0, \ldots, N-1$.

Equality (4.36) can now be used to rewrite the last set of equations appearing in (4.34) as

$$\begin{array}{l} \dfrac{d^{2m-1}\gamma}{dt^{2m-1}}(t_0^+) = \dfrac{(-1)^m}{\lambda}\big(p_0 - \gamma(t_0)\big) \\ \dfrac{d^{2m-1}\gamma}{dt^{2m-1}}(t_1^+) - \dfrac{d^{2m-1}\gamma}{dt^{2m-1}}(t_0^+) = \dfrac{(-1)^m}{\lambda}\big(p_1 - \gamma(t_1)\big) \\ \qquad\qquad \vdots \\ \dfrac{d^{2m-1}\gamma}{dt^{2m-1}}(t_{N-1}^+) - \dfrac{d^{2m-1}\gamma}{dt^{2m-1}}(t_{N-2}^+) = \dfrac{(-1)^m}{\lambda}\big(p_{N-1} - \gamma(t_{N-1})\big) \\ \qquad\qquad\quad - \dfrac{d^{2m-1}\gamma}{dt^{2m-1}}(t_{N-1}^+) = \dfrac{(-1)^m}{\lambda}\big(p_N - \gamma(t_N)\big) \end{array} . \tag{4.37}$$

Adding up both terms of the above system of equations, we obtain

$$\frac{(-1)^m}{\lambda}\sum_{i=0}^{N}\Big(p_i - \gamma(t_i)\Big) = 0, \tag{4.38}$$

which is equivalent to the first equation of the normal equations (4.32).

According to the explicit form (4.35) of the curve γ in each subinterval $\big[t_i, t_{i+1}\big]$, we can also write the last equation of (4.34) as

$$(2m-1)!\Big(a^i_{2m-1} - a^{i-1}_{2m-1}\Big) = \frac{(-1)^m}{\lambda}\big(p_i - \gamma(t_i)\big). \tag{4.39}$$

The corresponding condition for the derivative of γ of order $2m-2$ can also be written as

$$(2m-2)!\Big(a^i_{2m-2} - a^{i-1}_{2m-2}\Big) = -(2m-1)!t_i\Big(a^i_{2m-1} - a^{i-1}_{2m-1}\Big). \tag{4.40}$$

Plugging equation (4.39) into (4.40) and then summing up both terms of the previous $N+1$ equations, we conclude that

$$\frac{(-1)^m}{\lambda}\sum_{i=0}^{N} t_i\Big(p_i - \gamma(t_i)\Big) = 0,$$

which is equivalent to the second equation of (4.32).

To complete the proof, we claim that for $l \in \{2, \dots, m\}$, the condition fulfilled by the derivative of γ of order $2m - l$ is equivalent to

$$(l-1)!(2m-l)!\Big(a^i_{2m-l} - a^{i-1}_{2m-l}\Big) = (-1)^{l-1}(2m-1)!t_i^{l-1}\Big(a^i_{2m-1} - a^{i-1}_{2m-1}\Big). \tag{4.41}$$

If the above condition holds, then plugging (4.36) into (4.41) and then summing up those $N+1$ equations, we get

$$\frac{(-1)^m}{\lambda}\sum_{i=0}^{N} t_i^{l-1}\Big(p_i - \gamma(t_i)\Big) = 0,$$

for $l = 2, \dots, m$.

When λ goes to $+\infty$, we have already proved in proposition 3.2 (b), that the smoothing spline γ approaches an Euclidean polynomial of degree $m-1$. On the other hand, since the above $m-1$ equations together with equation (4.38) are equivalent to the normal equations (4.32), that Euclidean polynomial is therefore the solution of the classical least squares problem.

Let us assume that condition (4.41) holds for $l \in \{2, \dots, m-1\}$ and let us prove that it still holds for $l+1$.

The condition appearing in (4.34) for the derivative of γ of order $2m-l-1$ can be written as

$$(2m-l-1)!\Big(a^i_{2m-l-1} - a^{i-1}_{2m-l-1}\Big) + (2m-l)!\, t_i \Big(a^i_{2m-l} - a^{i-1}_{2m-l}\Big) +$$
$$+ \cdots + \frac{(2m-2)!}{(l-1)!}\, t_i^{l-1}\Big(a^i_{2m-2} - a^{i-1}_{2m-2}\Big) + \frac{(2m-1)!}{l!}\, t_i^{l}\Big(a^i_{2m-1} - a^{i-1}_{2m-1}\Big) = 0.$$

Now, if we use the induction step (4.41), we obtain after some manipulations

$$\begin{aligned} l!(2m-l-1)!\Big(a^i_{2m-l-1} - a^{i-1}_{2m-l-1}\Big) &= \\ &= -\sum_{j=1}^{l}(-1)^{l-j}\frac{l!}{(l-j)!j!}(2m-1)!\, t_i^{l}\Big(a^i_{2m-1} - a^{i-1}_{2m-1}\Big) \\ &= (-1)^{l+1}(2m-1)!\, t_i^{l}\Big(a^i_{2m-1} - a^{i-1}_{2m-1}\Big), \end{aligned}$$

† which finishes the proof. ∎

†To prove the last equality, we used the fact that $\sum_{j=0}^{l}(-1)^{l-j}\frac{l!}{(l-j)!j!} = 0$.

For the particular case when $m = 2$, we conclude from the previous theorem that the straight line obtained by the described limiting process is indeed the solution of the corresponding classical least squares problem, thus also generalizing the results appearing in [30] and in [24].

We finish with some illustrations in the plane $\mathbb{R}^2$ of the results presented here, for some specific data, where we can see that polynomials that are the solution of the classical least squares problems are obtained by this limiting process.

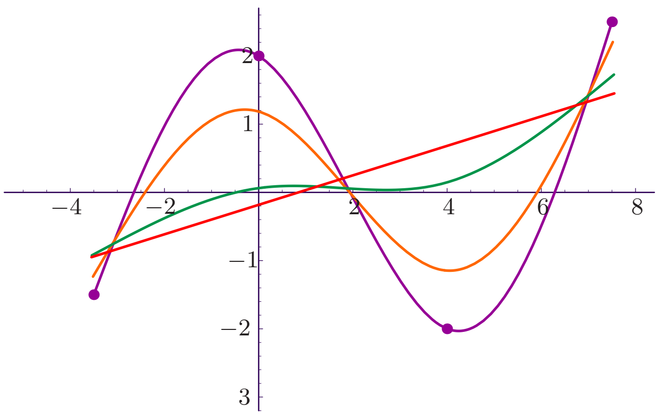

FIGURE 7. $q_0 = \left(-\frac{7}{2}, -\frac{3}{2}\right)$, $q_1 = (0, 2)$, $q_2 = (4, -2)$, $q_3 = \left(\frac{15}{2}, \frac{5}{2}\right)$, $t_0 = 0$, $t_1 = \frac{1}{3}$, $t_2 = \frac{2}{3}$ and $t_3 = 1$. The smoothing cubic splines were obtained for the following values of λ: $\lambda_1 = 10^{-5}$, $\lambda_2 = 10^{-3}$, $\lambda_3 = 10^{-2}$ and $\lambda_4 = 10$.

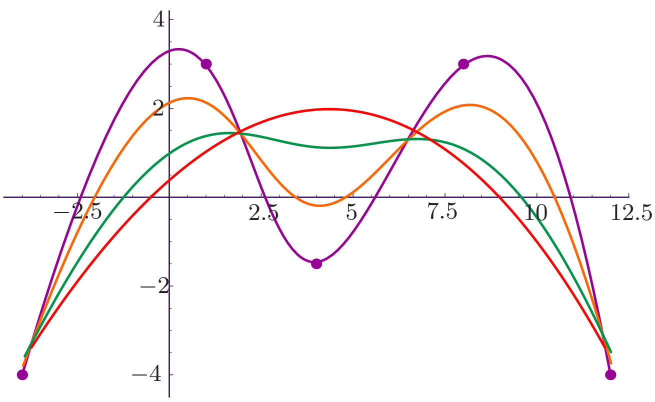

FIGURE 8. $q_0 = (-4, -4)$, $q_1 = (1, 3)$, $q_2 = \left(4, -\frac{3}{2}\right)$, $q_3 = (8, 3)$, $q_4 = (12, -4)$, $t_0 = 0$, $t_1 = \frac{1}{4}$, $t_2 = \frac{1}{2}$, $t_3 = \frac{3}{4}$ and $t_4 = 1$. The smoothing splines of degree 5 were obtained for the following values of λ: $\lambda_1 = 10^{-7}$, $\lambda_2 = 10^{-5.3}$, $\lambda_3 = 10^{-4.6}$ and $\lambda_4 = 10^3$.

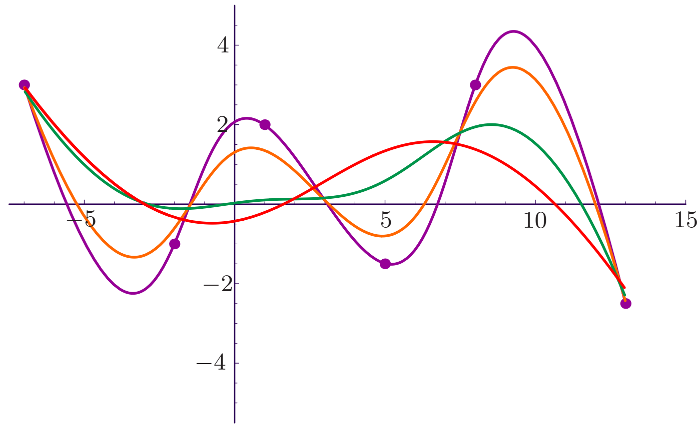

FIGURE 9. $q_0 = (-7, 3)$, $q_1 = (-2, -1)$, $q_2 = (1, 2)$, $q_3 = \left(5, -\frac{3}{2}\right)$, $q_4 = (8, 3)$, $q_5 = \left(13, -\frac{5}{2}\right)$, $t_0 = 0$, $t_1 = \frac{1}{5}$, $t_2 = \frac{2}{5}$, $t_3 = \frac{3}{5}$, $t_4 = \frac{4}{5}$ and $t_5 = 1$. The smoothing splines of degree 7 were obtained for the following values of λ: $\lambda_1 = 10^{-10}$, $\lambda_2 = 10^{-8}$, $\lambda_3 = 10^{-7}$ and $\lambda_4 = 10^{-4}$.

5. Conclusion

In this paper, we presented a generalization of high order classical least squares problems to more general Riemannian manifolds.

The formulation of the classical least squares problem given at the very beginning of section 4 has not a straightforward generalization to more general Riemannian manifolds. In fact, the non availability of explicit forms for the analogous to polynomial curves on manifolds was the main drawback to establish this generalization.

Nevertheless, the variational approach used to define such polynomial curves referred in subsection 2.2 enabled us to formulate in section 3 the variational problem $(\mathcal{P})$, depending on a smoothing parameter, and giving rise to what we call smoothing geometric splines.

These curves fit the given data and are obtained by piecing smoothly together segments of geometric polynomials. The Riemannian mean of the given points could also be obtained as a limiting process of those smoothing geometric splines, as it was proved in Theorem 3.3.

It was also possible to prove Theorem 4.1, that when the smoothing parameter goes to infinity, the smoothing geometric curves approach a smooth curve that turns out to be the solution of the classical least squares problem for the particular case when the manifold reduces to an Euclidean space.

These facts were illustrated in the plane $\mathbb{R}^2$ and in the sphere S^2, in figures 3-9, using the software Matlab 7.1 and Mathematica 5.1.

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