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THE GEOMETRIC MEAN AND THE GEODESIC FITTING PROBLEM ON THE GRASSMANN MANIFOLD

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ABSTRACT: The main objective of this paper is to solve the problem of finding a geodesic that best fits a given set of time-labelled points on the Grassmann manifold. To achieve this goal and derive the corresponding normal equations, we first deduce a formula for the geodesic arc joining two points on the Grassmannian, depending explicitly only on the given points. This allows to simplify the expression for the geodesic distance, which is crucial to generalize the best fitting problem, and is also used successfully to obtain a characterization of the geometric mean of a finite set of points lying on the Grassmannian, where the given points enter explicitly.

KEYWORDS: Grassmann manifold, geodesic distance, geometric mean, normal equations, fitting problems.

1. Introduction

The use of differential geometry notions and techniques to solve problems arising in physics and engineering has increased considerably in the past few years, due to the increasing awareness that using classical approaches to solve many of these problems leads to unsatisfactory results.

In this paper we generalize for the Grassmann manifold two classical problems of extreme importance within the scientific community, namely the geometric mean and the geodesic that best fits a finite collection of data points on the Grassmanian. These problems arise from a wide range of fields varying from artificial intelligence, image processing and pattern recognition to statistics or data mining. For concrete applications and examples of real problems where the geometry of the underlying spaces has been taken into account, we refer to [20], [25], [7], [19], [18] and [26]. As some of these examples illustrate, generalizing classical methods to curved spaces can be rather challenging. One of the difficulties, also presented here, is related to lack of existence and/or uniqueness of highly non-linear equations.

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The concept of center of mass for points lying on a Riemannian manifold appeared in the pioneer work of Karcher [14], in 1977. Since then, the generalization of the center of mass, hereafter called geometric mean or Riemannian mean, but often named Kacher mean in the literature, has been explored for a variety of Riemannian manifolds that play an important role in applications. We refer [5] for the spherical Kacher mean, [17] when the manifold is the rotation group, [18], [3] and [9], for data on the set of symmetric and positive definite tensors (the SPD manifold), and [13] and [23] concerning data on the Grassmann manifold.

The approach that we present here also includes the geometric mean for data on the Grassmannian. However, we take a step further when deriving an explicit characterization of the geodesic distance between two points. This allows to obtain a simplified expression to compute the geometric mean and, later, to compute the geodesic that best fits a set of data points, a generalization of the classical linear regression problem that has already been studied, in [16], when the manifold is the sphere or a connected and compact Lie group.

The organization of the paper is as follows. In section 2, we gather all the necessary information about the geometry of the Grassmann manifold that will be used to derive our main results. In particular, the Grassmannian is seen as an embedded submanifold of the manifold of symmetric matrices equipped with the Euclidean metric. In section 3, we exhibit the explicit expression for the geodesic distance on the Grassmannian with respect to such metric. This is the key-point to successfully derive in section 4 the equation that yields the geometric mean of a set of points in the Grassmannian. Finally, in section 5 we address the geodesic fitting problem on the Grassmannian and present the corresponding normal equations.

2. The geometry of the Grassmann manifold

The real Grassmann manifold $G_{n,k}$ is usually defined in Differential Geometry literature as the set of all $k-$dimensional linear subspaces of $\mathbb{R}^n$. It is a smooth and compact manifold of dimension $k(n-k)$. However, there is a diffeomorphism between the Grassmann manifold and the set of all symmetric projection operators of rank k ([8]), and this allows to look at $G_{n,k}$ as an embedding submanifold of the manifold consisting of all symmetric matrices of order n. This is the definition that we adopt here. But first, we introduce a few notations.

Let $\mathfrak{gl}(n)$ be the set of all $n \times n$ matrices with real entries, equipped with the Euclidean inner product

$$\langle X, Y \rangle = \mathrm{tr}\big(X^{\top} Y\big), \ \ X, Y \in \mathfrak{gl}(n). \tag{2.1}$$

The subset of $\mathfrak{gl}(n)$ of all symmetric matrices will be denoted by $\mathfrak{s}(n)$ and the subset of all skew-symmetric matrices by $\mathfrak{so}(n)$. It is well known that

$$\mathfrak{gl}(n) = \mathfrak{s}(n) \oplus \mathfrak{so}(n), \tag{2.2}$$

is a Cartan decomposition of the Lie algebra $\mathfrak{gl}(n)$. In particular, if $[.,.]$ denotes the usual commutator of matrices ($[A, B] = AB - BA$), one has

$$[\mathfrak{so}(n), \mathfrak{so}(n)] \subset \mathfrak{so}(n), \quad [\mathfrak{so}(n), \mathfrak{s}(n)] \subset \mathfrak{s}(n), \quad [\mathfrak{s}(n), \mathfrak{s}(n)] \subset \mathfrak{so}(n). \tag{2.3}$$

Also, $\mathfrak{so}(n)$ and $\mathfrak{s}(n)$ are orthogonal with respect to the inner product (2.1).

Throughout the paper, we adopt the following definition for the Grassmann manifold (or Grassmannian),

$$G_{n,k} := \big\{P \in \mathfrak{s}(n) \ : \ P^2 = P \text{ and } \mathrm{rank}(P) = k\big\}. \tag{2.4}$$

Smooth curves on $G_{n,k}$ can be parameterized explicitly by $\alpha(t) = \Theta(t) P \Theta(t)^T$, where Θ is a smooth curve on the orthogonal Lie group $O(n)$. In order to characterize the tangent space of $G_{n,k}$ at a point P, $T_P G_{n,k}$, one considers any smooth curve, $t \mapsto \alpha(t) = \Theta(t) P \Theta(t)^T$, satisfying $\alpha(0) = P$ and derives conditions for $\dot{\alpha}(0)$. Since $\Theta(0) = I$ and the tangent space of $O(n)$ at the identity I is $\mathfrak{so}(n)$, one has $\dot{\Theta}(0) = \Omega \in \mathfrak{so}(n)$, $\dot{\alpha}(0) = [\Omega, P]$, and, therefore,

$$T_P G_{n,k} = \big\{[\Omega, P] \ : \ \Omega \in \mathfrak{so}(n)\big\}. \tag{2.5}$$

It follows that the Riemannian metric induced by the Euclidean inner product (2.1) can be defined as

$$\langle [\Omega_1, P], [\Omega_2, P] \rangle = -\mathrm{tr}\big(\Omega_1 \Omega_2\big), \tag{2.6}$$

for $\Omega_1, \Omega_2 \in \mathfrak{so}(n)$.

For more details on the differential geometric structure of the Grassmannian, we refer to [6] and [1].

For P an arbitrary point in the Grassmannian $G_{n,k}$, define the following sets of matrices

$$\begin{aligned}
\mathfrak{gl}_P(n) &:= \{M \in \mathfrak{gl}(n) \ : \ M = PM + MP\};\\
\mathfrak{s}_P(n) &:= \mathfrak{s}(n) \cap \mathfrak{gl}_P(n);\\
\mathfrak{so}_P(n) &:= \mathfrak{so}(n) \cap \mathfrak{gl}_P(n).
\end{aligned}$$

Due to their interesting properties, listed below, these sets will play an important role in the next session about geodesics.

Lemma 2.1. *Let $P \in G_{n,k}$, $M \in \mathfrak{gl}_P(n)$ and $k \in \mathbb{N}$. Then the following holds.*

1. $PM^{2k-1}P = 0$;
2. $M^{2k-1} = PM^{2k-1} + M^{2k-1}P$;
3. $PM^{2k} = PM^{2k}P = M^{2k}P$;
4. $[P, [P, M]] = M$;
5. $M[M, P] = -[M, P]M$;
6. $(I - 2P)M = -M(I - 2P) = [M, P]$.

Proof: The first three properties can be proved by induction on k. However, in order to prove the inductive step of each one it is necessary to use the other identities when $k = 1$. So, our procedure will be to prove the first three properties for $k = 1$, and then complete the inductive step for the second property only, since the proof of the others use similar arguments.

The second assertion for $k = 1$ is true since $M \in \mathfrak{gl}_P(n)$. To prove that the first assertion holds for $k = 1$, replace M by the equivalent form $PM + MP$ in the expression PMP and use the fact that $P^2 = P$. Then,

$$\begin{aligned} PMP &= P(PM + MP)P \\ &= PMP + PMP, \end{aligned}$$

and the result follows. In order to prove that the third assertion holds for $k = 1$, also take into account that $PMP = 0$, to obtain

$$\begin{aligned} PM^2 &= P(PM + MP)(PM + MP) \\ &= (PM + PMP)(PM + MP) \\ &= PMPM + PM^2P \\ &= PM^2P. \end{aligned}$$

Analogously, it can be shown that $M^2P = PM^2P$.

We now prove the inductive step for the second property, that is, if $M^{2k-1} = PM^{2k-1} + M^{2k-1}P$, then $M^{2k+1} = PM^{2k+1} + M^{2k+1}P$. (Here we use the third assertion when $k = 1$).

$$\begin{aligned} M^{2k+1} &= M^2M^{2k-1} = M^2(PM^{2k-1} + M^{2k-1}P) = M^2PM^{2k-1} + M^{2k+1}P \\ &= PM^{2k+1} + M^{2k+1}P. \end{aligned}$$

We have completed the proof of the second assertion (if $M \in \mathfrak{gl}_P(n)$, then all odd powers of M belong to $\mathfrak{gl}_P(n)$).

The inductive steps for the other assertions are proved similarly, and the last three properties follow easily from the previous. For instance,

$$\begin{aligned} [P,[P,M]] &= (P(PM-MP)-(PM-MP)P) \\ &= PM - PMP - PMP + MP \\ &= PM + MP \\ &= M, \end{aligned}$$

which proves the fourth assertion. ■

This lemma can be used to prove that the restriction to $\mathfrak{gl}_P(n)$ of the adjoint operator at P

$$\begin{array}{rccc} \mathrm{ad}_P: & \mathfrak{gl}(n) & \longrightarrow & \mathfrak{gl}(n) \\ & M & \longmapsto & [P,M] \end{array}, \tag{2.7}$$

is an isometry.

Proposition 2.2. *Let $P \in G_{n,k}$. The adjoint operator $ad_P\Big|_{\mathfrak{gl}_P(n)} : \mathfrak{gl}_P(n) \to \mathfrak{gl}_P(n)$ is a global isometry.*

Proof: Assume that $M_1, M_2 \in \mathfrak{gl}_P(n)$. Then,

$$\begin{aligned} \langle \mathrm{ad}_P(M_1), \mathrm{ad}_P(M_2)\rangle &= \langle [P,M_1],[P,M_2]\rangle \\ &= \mathrm{tr}((\mathrm{M}_1^\top \mathrm{P} - \mathrm{P}\mathrm{M}_1^\top)(\mathrm{P}\mathrm{M}_2 - \mathrm{M}_2\mathrm{P})) \\ &= \mathrm{tr}(\mathrm{M}_1^\top\mathrm{P}\mathrm{M}_2 - \mathrm{M}_1^\top\mathrm{P}\mathrm{M}_2\mathrm{P} - \mathrm{P}\mathrm{M}_1^\top\mathrm{P}\mathrm{M}_2 + \mathrm{P}\mathrm{M}_1^\top\mathrm{M}_2\mathrm{P}) \\ &= \mathrm{tr}(\mathrm{M}_1^\top\mathrm{P}\mathrm{M}_2 + \mathrm{P}\mathrm{M}_1^\top\mathrm{M}_2) \\ &= \mathrm{tr}((\mathrm{P}\mathrm{M}_1 + \mathrm{M}_1\mathrm{P})^\top\mathrm{M}_2) \\ &= \mathrm{tr}(\mathrm{M}_1^\top\mathrm{M}_2) \\ &= \langle M_1, M_2\rangle, \end{aligned}$$

which proves that $\mathrm{ad}_P\Big|_{\mathfrak{gl}_P(n)}$ is a distance-preserving mapping.

It remains to prove that $\mathrm{ad}_P\Big|_{\mathfrak{gl}_P(n)}$ is bijective. For that, it is enough to show that if $M \in \mathfrak{gl}_P(n)$ is arbitrary, there exists a unique $N \in \mathfrak{gl}_P(n)$ such that $\mathrm{ad}_P(N) = M$. We show that $N := [P, M]$ satisfies such requirement. Since

$$\begin{aligned} PN + NP &= P[P,M] + [P,M]P = PM - PMP + PMP - MP \\ &= PM - MP \\ &= [P,M] \\ &= N, \end{aligned}$$

we have the guarantee that $N \in \mathfrak{gl}_P(n)$. So, from property *4.* of Lemma 2.1, it follows that $\mathrm{ad}_P([P,M]) = M$. To prove the uniqueness, assume that there exist $N_1, N_2 \in \mathfrak{gl}_P(n)$ such that $\mathrm{ad}_P(N_1) = \mathrm{ad}_P(N_2)$. But using again the same property, one concludes that $N_1 = N_2$. ■

Proposition 2.3. *Let $P \in G_{n,k}$. Then,*

1. $ad_P(\mathfrak{gl}(n)) = \mathfrak{gl}_P(n)$;
2. $ad_P(\mathfrak{s}(n)) = ad_P(\mathfrak{s}_P(n)) = \mathfrak{so}_P(n)$;
3. $ad_P(\mathfrak{so}(n)) = ad_P(\mathfrak{so}_P(n)) = \mathfrak{s}_P(n)$.

Proof: To prove the first assertion use the same arguments as for the proof of bijectivity of the adjoint operator at P used in the previous proposition.

The last two properties follow from the Cartan decomposition (2.2), together with the properties of the adjoint operator at P. ■

Remark 2.1. *Using previous considerations and propositions, together with some computations, leads to an alternative parameterization of the tangent space at a point $P \in G_{n,k}$:*

$$\begin{aligned} T_P G_{n,k} &= \mathfrak{s}_P(n) \\ &= \{ad_P^2(S) \ : \ S \in \mathfrak{s}(n)\} \\ &= \{ad_P(\Omega) : \Omega \in \mathfrak{so}_P(n)\}. \end{aligned} \tag{2.8}$$

Consequently, the normal space at P, with respect to the Euclidean metric, is defined by

$$T_P^{\perp} G_{n,k} = \{Z - ad_P^2(Z) \ : \ Z \in \mathfrak{s}(n)\} \tag{2.9}$$

We note that these descriptions of the tangent and normal spaces already appeared in [11].

3. Geodesics and geodesic distance

Proposition 3.1. *The unique geodesic $t \mapsto \gamma(t)$ in $G_{n,k}$, satisfying the initial conditions $\gamma(0) = P$ and $\dot\gamma(0) = [\Omega, P]$, where $\Omega \in \mathfrak{so}_P(n)$, is given by*

$$\gamma(t) = e^{t\Omega} P e^{-t\Omega}. \tag{3.10}$$

Proof: According to the above characterization of the normal space, it follows immediately that geodesics in $G_{n,k}$ are the solutions of the second order differential equation

$$[\gamma, [\gamma, \ddot\gamma]] = 0. \tag{3.11}$$

In order to prove the assertion, we first show that γ satisfies this differential equation if and only if $[\Omega, \mathrm{ad}_P^2(\Omega)] = 0$.

Differentiating (3.10) with respect to t, one gets $\dot\gamma(t) = [\Omega, \gamma(t)]$ and $\ddot\gamma(t) = [\Omega, [\Omega, \gamma(t)]]$. Now, using the Jacobi identity and the property *4.*, in Lemma 2.1, with $[\Omega, \gamma]$ instead of M, one can write:

$$\begin{aligned}
[\gamma, [\gamma, \ddot\gamma]] = 0 &\iff [\gamma, [\gamma, [\Omega, [\Omega, \gamma]]]] = 0 \\
&\iff [\gamma, [\Omega, [[\Omega, \gamma], \gamma]] + [\Omega, [[\Omega, \gamma], [\gamma, \Omega]] = 0 \\
&\iff [\Omega, [[\Omega, \gamma], \gamma], \gamma] + [[[\Omega, \gamma], \gamma], [\gamma, \Omega]] = 0 \\
&\iff [\Omega, \mathrm{ad}_\gamma^2([\Omega, \gamma])] - [\mathrm{ad}_\gamma^2(\Omega), [\Omega, \gamma]] = 0 \\
&\iff [\Omega - \mathrm{ad}_\gamma^2(\Omega), [\Omega, \gamma]] = 0 \\
&\iff [\Omega, \mathrm{ad}_\gamma^2(\Omega)] = 0.
\end{aligned}$$

The last equivalence may not seem obvious, but it can be easily checked if the operator ad_γ is applied to each one of the equations involved. But it also happens that

$$[\Omega, \mathrm{ad}_\gamma^2(\Omega)] = 0 \iff [\Omega, \mathrm{ad}_P^2(\Omega)] = 0.$$

Now, it is enough to show that if $\Omega \in \mathfrak{so}_P(n)$, then the last identity is satisfied. But, it follows from property 4. of Lemma 2.1 that $\mathrm{ad}_P^2(\Omega) = [P, [P, \Omega] = \Omega$, and thus $[\Omega, \mathrm{ad}_P^2(\Omega)] = 0$.

■

We note that the geodesic equation (3.11) is equivalent to the following differential equation appearing in [13]:

$$\ddot\gamma + [\dot\gamma, [\dot\gamma, \gamma]] = 0.$$

To check this equivalence it is enough to use the Jacobi identity.

We also need the following extra properties.

Lemma 3.2. *For $P \in G_{n,k}$ and $M \in \mathfrak{gl}_P(n)$, the following identities hold:*

1. $\sinh M = P \sinh M + \sinh M\, P$;
2. $P \sinh M\, P = 0$;
3. $\cosh M\, P = P \cosh M = P \cosh M\, P$;
4. $e^M P - P e^{-M} = \sinh M$.

Proof: To conclude that the first three properties hold, it is enough to apply Lemma 2.1, after noticing that

$$\mathrm{e}^M = \sinh M + \cosh M,$$

where $\sinh M$ and $\cosh M$ are defined through the Taylor series expansions

$$\sinh M = \sum_{n=0}^{+\infty} \frac{M^{2n+1}}{(2n+1)!} \text{ and } \cosh M = \sum_{n=0}^{+\infty} \frac{M^{2n}}{(2n)!}.$$

The last property follows from the previous, since

$$\begin{aligned} \mathrm{e}^M P - P\mathrm{e}^{-M} &= \cosh M\, P + \sinh M\, P - P \cosh M + P \sinh M \\ &= P \cosh M + \sinh M\, P - P \cosh M + P \sinh M \\ &= \sinh M. \end{aligned}$$

■

In order to obtain the geodesic distance between points P and Q in the Grassmannian $G_{n,k}$, we need to solve the equation $\mathrm{e}^{\Omega} P \mathrm{e}^{-\Omega} = Q$ with respect to Ω. The next theorem is the main result of this section. In order to understand the restrictions put on P and Q in the statement below, we recall that if a nonsingular matrix Y has no negative real values, then there exists a unique matrix A such that $\mathrm{e}^A = Y$ and whose spectrum lies in the horizontal strip $\{z \in \mathbb{C} : -\pi < \mathrm{Im}(z) < \pi\}$, [10]. This unique matrix A is called the principal logarithm of Y and we write $A = \log Y$. In the following, I denotes the $n \times n$ identity matrix.

Theorem 3.3. *Let $P, Q \in G_{n,k}$ and let $\Omega \in \mathfrak{so}_P(n)$ be such that $Q = e^{\Omega} P e^{-\Omega}$. Then*

$$\Omega = \frac{1}{2} \log((I - 2Q)(I - 2P)). \tag{3.12}$$

Proof: Before starting the proof, notice that we are assuming that P and Q can be joined by a geodesic. So, there is an implicit condition on these two matrices, namely that the orthogonal matrix $(I-2P)(I-2Q)$ has no negative real eigenvalues.

Using the last identity in Lemma 3.2, we can write the following identities

$$\begin{aligned} e^{\Omega}Pe^{-\Omega} &= (\sinh\Omega + Pe^{-\Omega})e^{-\Omega} \\ &= \left(\tfrac{1}{2}(e^{\Omega}-e^{-\Omega}) + Pe^{-\Omega}\right)e^{-\Omega} \\ &= Pe^{-2\Omega} + \tfrac{1}{2}I - \tfrac{1}{2}e^{-2\Omega}. \end{aligned}$$

Therefore,

$$e^{\Omega}Pe^{-\Omega} = Q \iff (P - \tfrac{1}{2}I)e^{-2\Omega} = Q - \tfrac{1}{2}I$$

Solving the above equation for Ω and taking into account that $2P-I$ is orthogonal yields the result. ■

Taking into account Theorem 3.3, the minimizing geodesic with respect to the Riemannian metric (2.6) that joins P, at $t=0$, to Q, at $t=1$, is parameterized explicitly by

$$\gamma(t) = e^{\frac{t}{2}\log((I-2Q)(I-2P))}Pe^{-\frac{t}{2}\log((I-2Q)(I-2P))}, \tag{3.13}$$

and thus the geodesic distance between points P and Q is given by

$$d^2(P,Q) = -\frac{1}{4}\mathrm{tr}\left(\log^2((I-2Q)(I-2P))\right). \tag{3.14}$$

Before proceeding, we recall some important properties of the matrix exponential and logarithm. The first property that we would like to point out is the fact that, for any non-singular matrices A and B, for which $\log B$ is defined, we have [10],

$$A^{-1}(\log B)A = \log\left(A^{-1}BA\right).$$

Next, we recall some results concerning the derivative of the exponential and the logarithm mappings that will be very useful in the next sections.

Lemma 3.4. ([21], [24]) *If $t \longmapsto X(t)$ is a differentiable function in $\mathfrak{gl}(n)$, then*

$$\frac{d}{dt}\exp X(t) = \left.\frac{e^u-1}{u}\right|_{u=\mathrm{ad}_{X(t)}}\left(\dot{X}(t)\right)\exp\left(X(t)\right),$$

where $\dfrac{e^u-1}{u}$ denotes the sum of the series $\displaystyle\sum_{m=0}^{+\infty}\frac{u^m}{(m+1)!}$.

Now, if we differentiate with respect to t the identity $\mathrm{e}^{\log Y(t)} = Y(t)$, we obtain the corresponding expression for the derivative of the matrix logarithm .

Lemma 3.5. *If $t \longmapsto Y(t)$ is a differentiable map such that $\log Y(t)$ is defined for all t, then*

$$\frac{d}{dt}\log Y(t) = \left.\frac{u}{\mathrm{e}^u - 1}\right|_{u=\mathrm{ad}_{\log Y(t)}} \big(\dot{Y}(t)Y^{-1}(t)\big),$$

where $\frac{u}{\mathrm{e}^u - 1}$ *denotes the sum of the series* $\displaystyle\sum_{m=0}^{+\infty} \frac{(-1)^m}{m+1}(\mathrm{e}^u - 1)^m$.

The next result states that, for $X \in \mathfrak{so}(n)$, the operator $\left.\frac{u}{\mathrm{e}^u - 1}\right|_{u=\mathrm{ad}_X}$ is skew-adjoint with respect to the inner product (2.1).

Lemma 3.6. *If $X \in \mathfrak{so}(n)$ and A, $B \in \mathfrak{gl}(n)$, then*

$$\left\langle \left.\frac{u}{\mathrm{e}^u - 1}\right|_{u=\mathrm{ad}_X}(A), B\right\rangle = \left\langle A, \left.\frac{u}{1 - \mathrm{e}^{-u}}\right|_{u=\mathrm{ad}_X}(B)\right\rangle.$$

4. The Riemannian mean in $G_{n,k}$

Let us recall that the geometric or Riemannian mean of a finite set of points $P_0, \ldots, P_N$ on a geodesically complete Riemannian manifold M, is a point belonging to M that minimizes the sum of its squared distances to the given points. When the manifold M is not geodesically complete, this definition requires that we restrict the optimization problem to a geodesically convex open set in M, similarly to what is usually required (see, for instance [13]).

So, according to the explicit expression for the geodesic distance in the Grassmannian $G_{n,k}$ given by (3.14), it is now straightforward to give a characterization of the mean for a finite set of points in $G_{n,k}$, belonging to a geodesically convex open ball $\mathcal{B} \subset G_{n,k}$.

Theorem 4.1. *Let $P_0, \ldots, P_N$ be a finite collection of points in $\mathcal{B} \subset G_{n,k}$. Then, P is a critical point for the function*

$$\begin{array}{rccl} \Phi: & \mathcal{B} & \to & \mathbb{R} \\ & P & \to & \Phi(P) = \sum_{i=0}^{N} d^2(P, P_i) \end{array}, \tag{4.15}$$

where d is the geodesic distance defined by (3.14), if and only if

$$\sum_{i=0}^{N} \log((I-2P)(I-2P_i)) = 0. \tag{4.16}$$

Proof: For the proof, one just needs to compute the tangent map of Φ at P. For that, consider a geodesic curve in $G_{n,k}$, $t \mapsto \gamma(t)$, satisfying $\gamma(0) = P$ and $\dot{\gamma}(0) = [X, P]$, where $X \in \mathfrak{so}_P(n)$. Then,

$$\begin{aligned}
&\big(d\Phi\big)_P([X,P]) = \\
&= \frac{d}{dt}\Big|_{t=0} \Phi\big(\gamma(t)\big) \\
&= -\frac{1}{4}\sum_{i=0}^{N} \frac{d}{dt}\Big|_{t=0} \operatorname{tr}\big(\log^2((I-2\gamma(t))(I-2P_i))\big) \\
&= \frac{1}{4}\sum_{i=0}^{N} \frac{d}{dt}\Big|_{t=0} \Big\langle \log((I-2\gamma(t))(I-2P_i)), \log((I-2\gamma(t))(I-2P_i)) \Big\rangle \\
&= -\frac{1}{2}\sum_{i=0}^{N}\Big\langle \frac{u}{\mathrm{e}^u - 1}\Big|_{u=\mathrm{ad}_{\log((I-2P)(I-2P_i))}} (2[X,P](I-2P)), \log((I-2P)(I-2P_i)) \Big\rangle.
\end{aligned}$$

Now, attending to the fact that for each $i = 0, \ldots, N$, $\log((I-2P)(I-2P_i)) \in \mathfrak{so}_P(n)$, using Lemma 3.6 together with property 6. of Lemma 2.1, the above expression is equivalent to

$$\begin{aligned}
\big(d\Phi\big)_P([X,P]) &= \sum_{i=0}^{N} \Big\langle X, \log((I-2P)(I-2P_i)) \Big\rangle \\
&= \Big\langle \big[X,P\big], \big[\sum_{i=0}^{N} \log((I-2P)(I-2P_i)), P\big] \Big\rangle.
\end{aligned}$$

Therefore, P is a critical point of Φ if and only if

$$\big(d\Phi\big)_P([X,P]) = 0, \ \forall X \in \mathfrak{so}(n),$$

that is, if and only if

$$\sum_{i=0}^{N} \log((I-2P)(I-2P_i)) = 0.$$

■

According to the above theorem, the gradient of the function Φ at P, that is, the unique vector field in $\mathcal{B} \subset G_{n,k}$, $(\nabla\Phi)(P)$, that satisfies

$$\big(d\Phi\big)_P([X,P]) = \Big\langle [X,P], (\nabla\Phi)(P)\Big\rangle, \ \ \forall X \in \mathfrak{so}(n),$$

is given by

$$(\nabla\Phi)(P) = \Big[\sum_{i=0}^{N} \log((I-2P)(I-2P_i)), P\Big].$$

If one compares the condition (4.16) in Theorem 4.1 with condition (33) in [13], it is not immediate to conclude that they are equivalent. But indeed they are. To see that, define Ω_i for $i = 0, \cdots, N$, as

$$\Omega_i := \log((I-2P)(I-2P_i)),$$

so that condition (4.16) reads as $\sum_{i=0}^{N} \Omega_i = 0$. The initial velocity of the geodesic joining P to P_i is $[\Omega_i, P]$ while the initial velocity of the geodesic joining P_i to P is $\xi_i := -[\Omega_i, P_i]$. The condition (33) in [13] is $\sum_{i=0}^{N} \xi_i = 0$. This, together with the fact that the geodesic distance is symmetric, is enough to conclude that both results are equivalent.

We turn now to the question of how to identify a local minima for the function Φ. For that, one has to study the second order optimality conditions that are based in the computation of the Riemannian Hessian. The Hessian of a function Φ at a critical point P, $(\mathrm{Hess}\,\Phi)_P$, is defined as in [2], by

$$\frac{d^2}{dt^2}\bigg|_{t=0} \Phi\big(\gamma(t)\big) = \Big\langle [X,P], (\mathrm{Hess}\,\Phi)_P([X,P])\Big\rangle.$$

The next result completely characterizes the Riemannian Hessian of the function Φ, defined by (4.15) at a point P satisfying (4.16).

Theorem 4.2. *The Riemannian Hessian of the function Φ, defined by $\Phi(P) = -\frac{1}{4}\sum_{i=0}^{N} tr\big(\log^2((I-2P)(I-2P_i))\big)$, at a critical point P, is given by*

$$(\mathrm{Hess}\,\Phi)_P([X,P]) = 2\Big[\sum_{i=0}^{N} \Big(\frac{u}{2}\coth\frac{u}{2}\Big)\Big|_{u=\mathrm{ad}_{\log((I-2P)(I-2P_i))}} (X), P\Big],$$

where $X \in \mathfrak{so}_P(n)$.

Proof: To compute the Riemannian Hessian of Φ at a critical point P, $(\operatorname{Hess}\Phi)_P$, let γ be a geodesic in $G_{n,k}$ satisfying $\gamma(0) = P$ and $\dot\gamma(0) = [X, P]$, where $X \in \mathfrak{so}_P(n)$. Thus, $\dot\gamma(t) = [X, \gamma(t)]$ and $\ddot\gamma(t) = [X, [X, \gamma(t)]]$. Therefore, introducing the notation

$$\Omega_i(t) = \log((I - 2\gamma(t))(I - 2P_i)),$$

and using the considerations above, we can write the following identities

$$\begin{aligned}
\frac{d}{dt}\Phi\big(\gamma(t)\big) &= \frac{1}{2}\sum_{i=0}^{N}\Big\langle \frac{d}{dt}\Omega_i(t), \Omega_i(t)\big)\Big\rangle \\
&= -\sum_{i=0}^{N}\Big\langle \frac{u}{\mathrm{e}^u - 1}\Big|_{u=\mathrm{ad}_{\Omega_i(t)}}\big([X, \gamma(t)](I - 2\gamma(t)))\big), \Omega_i(t)\Big\rangle \\
&= -\sum_{i=0}^{N}\Big\langle [X, \gamma(t)](I - 2\gamma(t)), \frac{u}{1 - \mathrm{e}^{-u}}\Big|_{u=\mathrm{ad}_{\Omega_i(t)}}\big(\Omega_i(t)\big)\Big\rangle \\
&= -\sum_{i=0}^{N}\Big\langle [X, \gamma(t)](I - 2\gamma(t)), \Omega_i(t)\Big\rangle.
\end{aligned}$$

Now, differentiate again the above expression with respect to t and then evaluate the result at $t = 0$, yields

$$\begin{aligned}
&\frac{d^2}{dt^2}\Big|_{t=0}\Phi\big(\gamma(t)\big) = \\
&= -\sum_{i=0}^{N}\frac{d}{dt}\Big|_{t=0}\Big\langle [X, \gamma(t)](I - 2\gamma(t)), \Omega_i(t)\big)\Big\rangle \\
&= \sum_{i=0}^{N} -\Big\langle [X, [X, P]](I - 2P), \Omega_i(0)\big)\Big\rangle + 2\Big\langle [X, P][X, P], \Omega_i(0)\Big\rangle \\
&\qquad + 2\Big\langle [X, P](I - 2P), \frac{u}{\mathrm{e}^u - 1}\Big|_{u=\mathrm{ad}_{\Omega_i(0)}}\big([X, P](I - 2P)\big)\Big\rangle
\end{aligned}$$

$$
\begin{aligned}
&= \sum_{i=0}^{N} -\Big\langle [X,[X,P]](I-2P), \Omega_i(0)\big) \Big\rangle + 2\Big\langle [X,P][X,P], \Omega_i(0) \Big\rangle \\
&+ 2\Big\langle X, \frac{u}{\mathrm{e}^u - 1}\bigg|_{u=\mathrm{ad}_{\Omega_i(0)}} (X) \Big\rangle,
\end{aligned} \tag{4.17}
$$

where the last equality follows from the fact that $[X,P](I-2P) = -X$. Taking now into account properties 5. and 6. of Lemma 2.1, we can write

$$
\begin{aligned}
[X,[X,P]](I-2P) &= X[X,P](I-2P) - [X,P]X(I-2P) \\
&= -[X,P]X(I-2P) - [X,P]X(I-2P) \\
&= -2[X,P]X(I-2P) \\
&= 2[X,P][X,P].
\end{aligned}
$$

Therefore, the first two expressions in (4.17) cancel out. Also, using the identity

$$
\frac{u}{\mathrm{e}^u - 1} = -\frac{u}{2} + \frac{u}{2}\coth\frac{u}{2},
$$

where

$$
\frac{u}{2}\coth\frac{u}{2} = 1 + \sum_{m=1}^{+\infty} \frac{\beta_{2m}}{(2m)!} u^{2m},
$$

and β_{2m} are Bernoulli numbers [4], the last expression in (4.17) is still equivalent to

$$
\begin{aligned}
&2\Big\langle X, \frac{u}{\mathrm{e}^u - 1}\bigg|_{u=\mathrm{ad}_{\Omega_i(0)}} (X) \Big\rangle = \\
&= -\Big\langle X, \big[\Omega_i(0), X\big] \Big\rangle + 2\Big\langle X, \Big(\frac{u}{2}\coth\frac{u}{2}\Big)\Big|_{u=\mathrm{ad}_{\Omega_i(0)}} (X) \Big\rangle \\
&= 2\Big\langle X, \Big(\frac{u}{2}\coth\frac{u}{2}\Big)\Big|_{u=\mathrm{ad}_{\Omega_i(0)}} (X) \Big\rangle.
\end{aligned}
$$

Finally, taking into account that $\left(\frac{u}{2}\coth\frac{u}{2}\right)\Big|_{u=\mathrm{ad}_{\Omega_i(0)}} (X) \in \mathfrak{so}_P(n)$, we have

$$
\frac{d^2}{dt^2}\bigg|_{t=0} \Phi\big(\gamma(t)\big) = \Big\langle [X,P], \big[2\sum_{i=0}^{N} \Big(\frac{u}{2}\coth\frac{u}{2}\Big)\Big|_{u=\mathrm{ad}_{\Omega_i(0)}} (X), P\big] \Big\rangle,
$$

and the result follows. ∎

Remark 4.1. *Analogously to what has been stated in Hüper and Manton [12] for the Lie group $SO(n)$, when the eigenvalues of the skew-symmetric matrices $\log((I-2P)(I-2P_k))$, for $k=0,\dots,N$, are of the form $i\alpha$, where $\alpha \in \big(-\pi,\pi\big)$, the Hessian of Φ is always positive definite. It turns out that, for the optimization problem restricted to the geodesically convex open ball $\mathcal{B}$, the above spectral condition is always satisfied, according to the remarks made just before Theorem 3.3. So, condition (4.16) implicitly defines the minimum for the function Φ.*

In order to find approximate solutions for the geometric mean in the Grassmann manifold, numerical methods on Riemannian manifolds have to be put to use, [22]. The explicit expressions for the gradient and for the Hessian of the function Φ derived above can now be used to implement either gradient or Newton-like algorithms.

5. The geodesic fitting problem

The objective in this section is to solve the geodesic fitting problem for the Grassmann manifold.

Let us consider a set of $N+1$ time-labelled points in $\mathcal{B}\subset G_{n,k}$, (P_i,t_i), where we assume for simplicity that the instants of time $t_0,\dots,t_N$ form a monotone increasing partition of the unit time interval $[0,1]$. Our aim is to find out a parameterized geodesic in $G_{n,k}$, $[0,1]\ni t\mapsto \gamma(t)=\mathrm{e}^{t\Omega}P\mathrm{e}^{-t\Omega}$, where $\gamma(0)=P\in G_{n,k}$ and $\Omega\in\mathfrak{so}_P(n)$, that yields the minimum value for the functional

$$E(\gamma)=\sum_{i=0}^{N} d^2(P_i,\gamma(t_i)). \tag{5.18}$$

Notice that finding the local minimizer γ for E is equivalent to finding the pair $(P,\Omega)\in G_{n,k}\times\mathfrak{so}_P(n)$ that minimizes the function F, defined by

$$F(P,\Omega){:=}\tfrac{1}{4}\sum_{i=0}^{N}\Big\langle\log((I-2\mathrm{e}^{t_i\Omega}P\mathrm{e}^{-t_i\Omega})(I-2P_i)),\log((I-2\mathrm{e}^{t_i\Omega}P\mathrm{e}^{-t_i\Omega})(I-2P_i))\Big\rangle. \tag{5.19}$$

In order to find the necessary optimality conditions, consider a smooth curve in $G_{n,k}$, $s\mapsto P(s)$ such that $P(0)=P$ and $\dot P(0)=S$, where $S\in\mathfrak{s}_P(n)$ and a smooth curve in $\mathfrak{so}_P(n)$, $s\mapsto\Omega(s)$ satisfying $\Omega(0)=\Omega$ and $\dot\Omega(0)=X$, with $X\in\mathfrak{so}_P(n)$.

For the sake of simplicity, let us introduce the notation

$$L_i(s) = \log((I - 2\mathrm{e}^{t_i\Omega(s)}P(s)\mathrm{e}^{-t_i\Omega(s)})(I - 2P_i)).$$

According to (3.13), notice that $\frac{1}{2}[\gamma(t_i), L_i(0)]$ is the velocity vector of the minimizing geodesic joining $\gamma(t_i)$ to P_i. So, taking into account property 6. of Lemma 2.1, we have

$$\big[\gamma(t_i), L_i(0)(I - 2\gamma(t_i))\big] = L_i(0).$$

Using Lemma 3.5, we can write

$$\begin{aligned}
&\left.\frac{d}{ds}\right|_{s=0} L_i(s) = \\
&= \left.\frac{u}{\mathrm{e}^u - 1}\right|_{u=\mathrm{ad}_{L_i(0)}} \Big(\big(\left.\frac{d}{ds}\right|_{s=0} \big(I - 2\mathrm{e}^{t_i\Omega(s)}P(s)\mathrm{e}^{-t_i\Omega(s)})\big)(I - 2\gamma(t_i))\Big),
\end{aligned}$$

and from Lemma 3.4, we still have

$$\begin{aligned}
&\left.\frac{d}{ds}\right|_{s=0} \big(I - 2\mathrm{e}^{t_i\Omega(s)}P(s)\mathrm{e}^{-t_i\Omega(s)})\big) = \\
&= -2\left.\frac{\mathrm{e}^u - 1}{u}\right|_{u=\mathrm{ad}_{t_i\Omega}} (t_iX)\gamma(t_i) - 2\gamma(t_i)\left.\frac{1 - \mathrm{e}^{-u}}{u}\right|_{u=\mathrm{ad}_{-t_i\Omega}} (-t_iX) - 2\mathrm{e}^{t_i\Omega}S\mathrm{e}^{-t_i\Omega} \\
&= -2\Big[\left.\frac{\mathrm{e}^u - 1}{u}\right|_{u=\mathrm{ad}_{t_i\Omega}} (t_iX), \gamma(t_i)\Big] - 2\mathrm{e}^{t_i\Omega}S\mathrm{e}^{-t_i\Omega}.
\end{aligned}$$

Therefore,

$$\begin{aligned}
&(dF)_{(P,\Omega)}(S,X) = \left.\frac{d}{ds}\right|_{s=0} F\big(P(s), \Omega(s)\big) = \frac{1}{2}\sum_{i=0}^{N}\Big\langle \left.\frac{d}{ds}\right|_{s=0} L_i(s), L_i(0)\Big\rangle \\
&= \frac{1}{2}\sum_{i=0}^{N}\Big\langle \big(\left.\frac{d}{ds}\right|_{s=0} (I - 2\mathrm{e}^{t_i\Omega(s)}P(s)\mathrm{e}^{-t_i\Omega(s)})\big)(I - 2\gamma(t_i)), L_i(0)\Big\rangle \\
&= -\sum_{i=0}^{N}\Big\langle \Big(\Big[\left.\frac{\mathrm{e}^u - 1}{u}\right|_{u=\mathrm{ad}_{t_i\Omega}} (t_iX), \gamma(t_i)\Big] + \mathrm{e}^{t_i\Omega}S\mathrm{e}^{-t_i\Omega}\Big)(I - 2\gamma(t_i)), L_i(0)\Big\rangle
\end{aligned}$$

$$
\begin{aligned}
&= -\sum_{i=0}^{N}\Big\langle \Big[\frac{\mathrm{e}^{u}-1}{u}\Big|_{u=\mathrm{ad}_{t_i\Omega}}(t_iX),\gamma(t_i)\Big](I-2\gamma(t_i)), L_i(0)\Big\rangle \\
&\quad -\sum_{i=0}^{N}\Big\langle \mathrm{e}^{t_i\Omega}S\mathrm{e}^{-t_i\Omega}(I-2\gamma(t_i)), L_i(0)\Big\rangle \\
&= -\sum_{i=0}^{N}\Big\langle \Big[\frac{\mathrm{e}^{u}-1}{u}\Big|_{u=\mathrm{ad}_{t_i\Omega}}(t_iX),\gamma(t_i)\Big], L_i(0)(I-2\gamma(t_i))\Big\rangle \\
&\quad -\sum_{i=0}^{N}\Big\langle \mathrm{e}^{t_i\Omega}S\mathrm{e}^{-t_i\Omega}, L_i(0)(I-2\gamma(t_i))\Big\rangle \\
&= -\Big\langle X, \sum_{i=0}^{N} t_i\,\frac{1-\mathrm{e}^{-u}}{u}\Big|_{u=\mathrm{ad}_{t_i\Omega}}\Big(\big[\gamma(t_i), L_i(0)(I-2\gamma(t_i))\big]\Big)\Big\rangle \\
&\quad - \Big\langle S, \sum_{i=0}^{N}\mathrm{e}^{-t_i\Omega}L_i(0)(I-2\gamma(t_i))\mathrm{e}^{t_i\Omega}\Big\rangle \\
&= -\Big\langle X, \sum_{i=0}^{N} t_i\,\frac{1-\mathrm{e}^{-u}}{u}\Big|_{u=\mathrm{ad}_{t_i\Omega}}\big(L_i(0)\big)\Big\rangle - \Big\langle S, \sum_{i=0}^{N}\mathrm{e}^{-t_i\Omega}L_i(0)(I-2\gamma(t_i))\mathrm{e}^{t_i\Omega}\Big\rangle.
\end{aligned}
\tag{5.20}
$$

Theorem 5.1. *A necessary condition for the geodesic $t \mapsto \gamma(t) = e^{t\Omega}Pe^{-t\Omega}$ to be a minimizer for the functional E, defined by (5.18), is that the pair $(P,\Omega) \in G_{n,k} \times \mathfrak{so}_P(n)$ satisfies the following system of equations*

$$
\begin{cases}
\displaystyle\sum_{i=0}^{N}\log\big((I-2P)(I-2\,\mathrm{e}^{-t_i\Omega}P_i\,\mathrm{e}^{t_i\Omega})\big) = 0 \\
\displaystyle\sum_{i=0}^{N} t_i\,\frac{\mathrm{e}^{u}-1}{u}\Big|_{u=\mathrm{ad}_{t_i\Omega}}\Big(\log\big((I-2P)(I-2\,\mathrm{e}^{-t_i\Omega}P_i\,\mathrm{e}^{t_i\Omega})\big)\Big) = 0
\end{cases}
. \tag{5.21}
$$

Proof: By definition, (P,Ω) is a critical point of F, defined by (5.19) if and only if

$$
\big(dF\big)_{(P,\Omega)}(S,X) = 0, \quad \forall (S,X) \in \mathfrak{s}_P(n) \times \mathfrak{so}_P(n). \tag{5.22}
$$

From the expression of the tangent map of F at point (P,Ω) given by (5.20), we conclude that condition (5.22) is equivalent to

$$\left\{\begin{array}{l}\displaystyle\sum_{i=0}^{N} \mathrm{e}^{-t_i\Omega} \log\left((I-2\gamma(t_i))(I-2P_i)\right)(I-2\gamma(t_i))\mathrm{e}^{t_i\Omega} = 0 \\ \displaystyle\sum_{i=0}^{N} t_i \left.\frac{1-\mathrm{e}^{-u}}{u}\right|_{u=\mathrm{ad}_{t_i\Omega}} \Big(\log\left((I-2\gamma(t_i))\,(I-2P_i)\right)\Big) = 0\end{array}\right. . \tag{5.23}$$

Now, the first equation of (5.23) can be rewritten as

$$\begin{aligned} 0 &= \sum_{i=0}^{N} \mathrm{e}^{-t_i\Omega} \log\big((I-2\,\mathrm{e}^{t_i\Omega}P\,\mathrm{e}^{-t_i\Omega})(I-2P_i)\big)\,(I-2\gamma(t_i))\mathrm{e}^{t_i\Omega} \\ &= \sum_{i=0}^{N} \mathrm{e}^{-t_i\Omega} \log\big((I-2\,\mathrm{e}^{t_i\Omega}P\mathrm{e}^{-t_i\Omega})(I-2P_i)\big)\,\mathrm{e}^{t_i\Omega}\mathrm{e}^{-t_i\Omega}(I-2\gamma(t_i))\mathrm{e}^{t_i\Omega} \\ &= \sum_{i=0}^{N} \log\big((I-2P)(I-2\mathrm{e}^{-t_i\Omega}P_i\mathrm{e}^{t_i\Omega})\big)\,(I-2P) \end{aligned}$$

and, therefore, it is equivalent to the first equation of (5.21).

Using similar techniques, it can be easily proven that the second equation of (5.23) is equivalent to the second equation of (5.21). ■

6. Conclusion remarks

After having derived the formula (3.14) for the geodesic distance between two points on the Grassmannanian, we have characterized the geometric mean of a finite set of points lying on the Grassmannian, only in terms of the given data (Theorem 4.1). We have also derived necessary conditions for the geodesic that solves the geodesic regression problem on the Grassmannian (Theorem 5.1).

Other generalizations of the classical least square problems can be formulated. One particular problem that stands up due to its importance in applications is that of finding the polynomial curve (degree greater than 1) that best fits a given data set. However, since no explicit expressions for geometric polynomials on Grassmann manifolds are known, the techniques used here, which are direct generalizations of the corresponding methods for $\mathbb{R}^n$, can't be applied. For these higher order problems on general manifolds, the variational approach presented in [15] may be used successfully as long as the Euler-Lagrange equations that characterize geometric polynomials on the Grassmannian are derived and could be solved, at least approximately. This is a very challenging problem that has not been solved yet even for simpler manifolds, since it requires methods of integration on manifolds that are not available.

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